NBS
PUBLICATIONS

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*NBS Special Publication 305*
*Supplement 18*

# *Publications of the National Bureau of Standards 1986 Catalog*

# PUBLICATIONS

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No.305
SUPPL.18
1987

*U.S. Department of Commerce*
*National Bureau of Standards*

The National Bureau of Standards[1] was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the Nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research to assure international competitiveness and leadership of U.S. industry, science and technology. NBS work involves development and transfer of measurements, standards and related science and technology, in support of continually improving U.S. productivity, product quality and reliability, innovation and underlying science and engineering. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, the Institute for Computer Sciences and Technology, and the Institute for Materials Science and Engineering.

## The National Measurement Laboratory

Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes Standard Reference Materials; provides calibration services; and manages the National Standard Reference Data System. The Laboratory consists of the following centers:

- Basic Standards[2]
- Radiation Research
- Chemical Physics
- Analytical Chemistry

## The National Engineering Laboratory

Provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

- Applied Mathematics
- Electronics and Electrical Engineering[2]
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering[3]

## The Institute for Comptuer Sciences and Technology

Conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following divisions:

- Information Systems Engineering
- Systems and Software Technology
- Computer Security
- Systems and Network Architecture
- Advanced Systems

## The Center for Materials Science

Conducts research and provides measurements, data, standards, reference materials, quantitative understanding and other technical information fundamental to the processing, structure, properties and performance of materials; addresses the scientific basis for new advanced materials technologies; plans research around cross-cutting scientific themes such as nondestructive evaluation and phase diagram development; oversees Bureau-wide technical programs in nuclear reactor radiation research and nondestructive evaluation; and broadly disseminates generic technical information resulting from its programs. The Institute consists of the following divisions:

- Ceramics
- Fracture and Deformation[3]
- Polymers
- Metallurgy
- Reactor Radiation

[1] Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg MD 20899
[2] Some divisions within the center are located at Boulder, CO 80303.
[3] Located at Boulder, CO with some elements at Gaithersburg, MD

Research Information Center
National Bureau of Standards
Gaithersburg, Maryland 20899

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# Publications of the National Bureau of Standards 1986 Catalog

Rebecca J. Pardee, Editor

Information Resources and Services Division
National Bureau of Standards
Gaithersburg, MD 20899

Issued June 1987

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Malcolm Baldrige, Secretary

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## CATALOG STRUCTURE AND USE

Full bibliographic citations including keywords and abstracts for National Bureau of Standards papers published and entered into the National Technical Information Service (NTIS) collection are cited in the "NBS Publications Announcements" section of this catalog. (Also included are NBS papers published prior to 1986 but not reported in previous supplements of this annual catalog.) Entries are arranged by NTIS subject classifications which consist of 38 broad subject categories (see back cover) and over 350 subcategories. Within a subcategory, entries are listed alphanumerically by NTIS order number.

Four additional abbreviated indexes are included to allow the user to identify NBS papers by personal author, keywords, title, and NTIS order/report number. Each entry lists the appropriate title, the NTIS order number, and the abstract number.

NBS papers may also be identified by searching the NTIS database either online via the commercially available DIALOG system or in the issues of NTIS's *Government Reports Announcements and Index* and its *Government Reports Annual Index*.

## AVAILABILITY AND ORDERING INFORMATION

The highest quality and least expensive copies of NBS publications published as Government documents are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. Publications cited with stock numbers (SN) and purchase orders should be cited by these numbers. GPO will accept payment by check, money order, VISA, Mastercharge, or deposit account. For availability and price, write to the GPO or telephone (202) 783-3258. Should an NBS publication be out of print at the GPO, its continued availability is assured at NTIS which sells publications in microfiche or paper copy reproduced from microfiche.

If an entry has a price code, such as PC A04/MF A01, the publication may be ordered from NTIS in paper copy (PC) or microfiche (MF) or both if both codes are given. Order from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. A copy of the latest price code schedule is available from NTIS. NTIS will accept payment by check, money order, VISA, American Express, Mastercharge, or deposit account, NTIS is the sole source of Federal Information Processing Standards (FIPS), NBS Interagency Reports (NBSIRs), and Grant/Contract Reports (GCRs).

Sometimes, papers noted "Not Available NTIS" may be obtained directly from the author or from the external publisher cited. Such papers are not for sale by either the GPO or NTIS.

Two other sources for NBS publications are depository libraries (libraries designated to receive Government publications) and Department of Commerce District Offices. The depository libraries listed in Appendix A receive selected NBS publications (see inside back cover for a description of the various NBS publication series). While not every Government publication is sent to all depository libraries, certain depositories designated as Regional Depositories receive and retain one copy of all Government publications made available. Contact the depository library in your area to obtain information on what is available and where.

Department of Commerce District Offices listed in Appendix B provide ready access at the local level to publications, statistical data and summaries, and surveys. Each District Office serves as an official sales agency of the Superintendent of Documents, U.S. Government Printing Office. A wide range of Government publications can be purchased from these offices. In addition, the reference library of each District Office contains review copies of many Government publications.

# NBS PUBLICATIONS ANNOUNCEMENTS

## *SAMPLE ENTRY*

**COMPUTERS, CONTROL & INFORMATION THEORY**

**NTIS Subject Category**

**Computer Software**
*500,320*
**PB86-167830** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Integrated Software for Microcomputer Systems**
L. S. Rosenthal. Jan. 86, 41p.
NBS/SP-500/135
Contract F-000000

**NTIS Subcategory**
*Abstract Number*
**NTIS order number** Availability **Price Codes**
Corporate or performing organization

**Report Title**
Personal authors Report date Page count
Report Number
Contract or grant number

Keywords: Microcomputers, *Computer software, *Integrated systems, . . .

Keywords: * indicates keyword index entry

Integrated software products combine several applications within a single program and enable information to be shared between the applications.

Abstract

# ADMINISTRATION & MANAGEMENT

### Management Information Systems

*600,001*
**PB86-247624** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Personal Computer Networks.**
Special pub. (Final),
J. Barkley. Jul 86, 62p NBS/SP-500/140
Also available from Supt. of Docs as SN003-003-02746-4. Library of Congress catalog card no. 86-600564.

Keywords: *Management information systems, Computer networks, Microcomputers, Surveys, Management, Administrative support, *Personal computers, *Office automation, End use.

The survey of personal computer network technology in today's office presents the point of view of the end user. It characterizes the capabilities of personal computer networks and the services which they provide the user in terms of generic features. As a result, technical management and end users will have an understanding of how personal computer networks can fit into an overall office automation strategy. The document does not discuss or evaluate alternatives for the sharing of data, such as, the manual exchange of floppy disks between personal computers.

### Management Practice

*600,002*
**PB85-106151** PC **A24**/MF **A01**
Toth (R.B.) Associates, McLean, VA.
**Standards Activities of Organizations in the United States.**
Final rept.,
R. B. Toth. Aug 84, 575p NBS/SP-681
Supersedes PB-249 542. Also available from Supt. of Docs. as SN003-02602-6. Library of Congress catalog card no. 84-601084.

Keywords: *Directories, *Organizations, *Management engineering, *Standardization, Standards, State government, National government, Technology, Social welfare, Criteria, United States, Private associations, Federal agencies.

This directory is a guide to mandatory and voluntary standards activities in the United States at Federal and state levels and by nongovernment (trade associations, technical and other professional societies). It excludes proprietary (company standards) and local levels of government (i.e., county and municipal). It supersedes the 1975 edition (NBS SP 417), 'Directory of United States Standardization Activities' and, for the first time, includes standards distributors, libraries, and information centers, and union lists of standards repositories by regional areas. It also lists organizations that no longer develop standards or have become defunct since the previous directory was issued. Over 750 current descriptive commentaries are formatted, with subject headings to facilitate access to specific information. The main sections cover nongovernment; Federal Government; state procurement offices; sources of standards documents and information; a subject index and related listings covering acronyms and initials, defunct bodies, and those organizations with name changes. Organizations have been included if they develop standards or contribute to the standardization process, whether voluntary or mandatory, or are sources of standards documents or information.

## Management Practice

An introductory section provides general information on Federal (including military) standards activities, a list of 20 major nongovernment standards developers, some historical notes, and an overview of U.S. (national) standardization activities.

*600,003*
**PB86-187705** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
**Advantages of the Adjusted Internal Rate of Return.**
Final rept.,
H. E. Marshall. Feb 86, 6p
Pub. in Jnl. of the American Association of Cost Engineers 28, n2 p32-37 Feb 86.

Keywords: *Budgeting, Economic analysis, Buildings, Project management, Reprints, Economic impact, *Adjusted internal rate of return, *Internal rate of return.

The internal rate of return is used frequently in evaluating the economic impacts of construction and other capital budgeting projects. Two versions of the internal rate of return are used. The first is the unadjusted internal rate of return (IRR), which has been most commonly used. It measures over the life of the project the return solely on the original investment, implying the same return on reinvestments of project cash flows as that earned on the original investment. The second less commonly used version, is the adjusted internal rate of return (AIRR). It measures over the life of the project the combined return on the original investment and on the reinvested earnings, allowing for the reinvestment rate(s) to differ from the rate earned on the original investment. The article defines IRR and AIRR; describes the controversy over which measure is better; compares methods for computing them; discusses assumptions implicit and explicit in their calculation; and describes the advantages of using AIRR instead of IRR. Appropriate applications of the AIRR and its limitations are also discussed.

*600,004*
**PB86-231305** PC **A04**/MF **A01**
Michigan Univ., Ann Arbor. Graduate School of Business Administration.
**Due-Date Based Scheduling in a Flexible Manufacturing System (The ATS),**
R. V. Rachamadugu, N. Raman, and F. B. Talbot.
Mar 86, 73p NBS/GCR-86/514
See also PB86-232402. Sponsored by National Bureau of Standards, Gaithersburg, MD.

Keywords: *Scheduling, Production planning, Automation, Optimization, *Flexible manufacturing systems, Computer aided manufacturing.

The paper is part of an ongoing project to develop a real-time scheduling system for the Automated Manufacturing Research Facility (AMRF) at the National Bureau of Standards in Gaithersburg, Maryland. It investigates the dynamic scheduling of the Automatic Turning Station (ATS) at the AMRF. The manufacturing characteristics of the ATS include processing of jobs in batches, and changeover times between jobs of different part types. The performance of the ATS is measured by mean flow time, mean tardiness, proportion of tardy jobs and standard deviation of tardiness.

*600,005*
**PB87-105276** PC **A09**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Revised Interim Design Guidelines for Automated Offices,**
A. I. Rubin. Aug 86, 179p NBSIR-86/3430
See also PB85-100410. Sponsored by General Services Administration, Washington, DC.

Keywords: *Office management, *Automation, Ergonomics, Design criteria, Organization theory, Office equipment, Environmental engineering, Workstations, Communication systems.

The report is an update of an earlier design guideline (NBSIR 84-2908). It is based upon an additional literature search and interviews. The information should still be considered tentative, since they are still based on judgement and practice, not formal studies. The introduction of automation into offices has changed the office as a workplace. Architects and other design professionals have responded to this technology by employing a number of design strategies. This report identifies design issues which merit consideration by the designer and suggests criteria and approaches that might be used in automated office design. Technological, ergonomic and organizational factors are all considered from the standpoint of their design implications. The present document is a major revision of the earlier study, including more than twice the number of reference documents than its predecessor.

## Personnel Management, Labor Relations & Manpower Studies

*600,006*
**AD-P002 923/1** PC **A02**/MF **A01**
National Bureau of Standards, Washington, DC.
**Vigilance Performance of Security Force Personnel,**
A. Ramey-Smith, and S. T. Margulis. 1 Jun 81, 9p
Pub. in Proceedings of the Symposium on the Role of Behavioral Science in Physical Security (5th Annual) Held at Gaithersburg, MD., June 11-12, 1980, AD-A138 882, p91-99.

Keywords: *Security personnel, *Performance(Human), *Behavioral science, Training, Vigilance, Management planning and control, Perception(Psychology), Response. Component Reports, Physical security.

The research being performed by the National Bureau of Standards (NBS) for the Defense Nuclear Agency (DNA) involves two tasks. Overall, its goal is to assess those factors that influence the individual state of vigilance in an effort to identify methods to improve this aspect of guard force performance on a daily and long term basis. The first task in achieving this goal is an investigation of the influences of the work environment on performance. That is, an evaluation will be performed of the factors related to the physical characteristics of the task that affect human behavior. This will involve a human engineering study of the vigilance task of security force personnel. The second task of this project is to study the influences of the social environment on a guard force performance. This aspect of the project will involve a social psychological and environmental study of the vigilance task. These two aspects of vigilance performance, that is, human engineering and social/environmental, are related. Both interact todefine the ultimate effectiveness of the guard's performance in a watchkeeping task. However, each is very broad in nature.

*600,007*
**PB86-196383** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
**Implementation Plan - Internal Revenue Service Strategic Intiatives ERR-9 and ERR-11.**
Rept. for Aug-Dec 85,
R. E. Schofer. Mar 86, 47p NBSIR-86/3336
Sponsored by Internal Revenue Service, Washington, DC.

Keywords: Implementation, Interviews, Recruiting, *Internal Revenue Service, Data collection, *Human resources, *Strategic planning.

The Internal Revenue Service (IRS) Strategic Plan is comprised of 55 Strategic Initiatives selected to prepare the Service for effective and efficient operation in the 1990's. Strategic Initiative ERR-9 addresses the development and use of a trend-analysis monitoring system for human resources planning; ERR-11 utilizes these data in development of recruitment plans for the Internal Revenue Service. The Phase-I Report presents the results of a review of human-resources planning requirements and a review of current research and development projects which impact human resources planning in the Internal Revenue Service. A ten-step plan for building and implementing a trend monitoring system for human resources planning is presented. The system also can be used to analyze operational issues which frequently must be addressed by the Personnel Division of IRS. The only recommendation for field collection of data pertains to a sample of exit interviews of departing employees and some interviews of first-line supervisors to measure attitudes. A bibliography is presented in the Appendix of the Report.

## Public Administration & Government

*600,008*
**PB87-114641** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Physical Measurement Services.
**National Bureau of Standards (NBS) Policy on the Use of Its Name in Advertising.**
Final rept.,
L. J. Kieffer. 1982, 2p
Pub. in NCSL Newsletter 22, n1 p12-13 Mar 82.

Keywords: *Advertising, Policies, Reprints, *National Bureau of Standards.

The information contained in NBS Letter Circular 1128, 'NBS Policy on Use of Its Name in Advertising,' is quoted. Additional information and discussion are presented to help explain and clarify the policy.

## Research Program Administration & Technology Transfer

*600,009*
**PB86-195211** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of the Director.
**Technology Policy Experiment as a Policy Research Tool.**
Final rept.,
G. Tassey. 1985, 14p
Pub. in Research Policy 14, n1 p39-52 1985.

Keywords: *Research projects, *Policies, *Technology, Regulations, Reprints, Industrial development.

The roles of the policy experiment are described and characterized as an important step in the industrial policy research process. The elements of the policy experiment are identified and the steps described by which an experiment is conducted and the results integrated into the overall policy research process. The importance of experimentation is emphasized for the effective development, implementation, and evaluation of industrial growth policies for technology-based industries. A case study of a policy experiment with new analytical and institutional procedures for monitoring the impacts of venture capital market regulations is used to show how the policy experiment can provide the necessary iterative and low-risk, low-cost approach to policy change. Equally important, institutionalization of the procedures for monitoring existing policies and the provision of decision-relevant information are shown to be important benefits from policy experimentation in the context of the overall policy change process.

*600,010*
**PB87-104741** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Public Information Div.
**NBS (National Bureau of Standards) Research Reports, July 1986.**
Jul 86, 37p NBS/SP-719
See also PB83-132704. Library of Congress catalog card no. 86-600556.

Keywords: *Research projects, National Bureau of Standards.

Contents: Research update; Spirit of cooperation alive and well at National Bureau of Standards; Taking the earth's measure at a unique institution; Gravity, when you get right down to it; The light fantastic; Safer, quicker ways to prepare samples for chemical analysis; Researchers study the process to improve measurement accuracy; Expanded version of IGES standard available; NBS studying new techniques to identify irradiated foods; NBS research in biotechnology: Providing the scientific fundamentals; New publications; Conference calendar.

# AERONAUTICS & AERODYNAMICS

## Aerodynamics

*600,011*
**PB87-122347** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Effect of Shear Layer Instabilities and Acoustic Modes on Vortex Formation in a Coflowing Jet.**
Final rept.,
J. M. McMichael, L. P. Purtell, R. W. Davis, and E. F. Moore. 1984, 7p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Proceedings of American Institute of Aeronautics and Astronautics Aerospace Sciences Meeting (2nd), Reno, NV., January 9-12, 1984, 7p.

Keywords: *Vortices, *Jets, Acoustics, Shear layers, Instability.

The early development of a circular jet issuing into a coflowing stream has been examined by hot-wire measurements and smoke-wire visualization. Linear stability theory has been found adequately to predict the response of the early shear layer to upstream disturbances. Knowing the exact nature of these disturbances (acoustic modes in the present case) is of utmost importance in understanding the character of oscillations in the shear layer and their subsequent evolution into vortical motions. It has been found that the coflowing stream has little influence on the stability characteristics of the early shear layer. On the other hand, the 'inner' shear layer (the remains of the inner boundary layer) strongly influences the stability characteristics. The response of the vortex development to controlled excitation has been found to be quite similar to that of the plane mixing layer provided that acoustic effects are taken into account.

## Test Facilities & Equipment

*600,012*
**PB87-127932** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.
**Surface Roughness Studies for Wind Tunnel Models Used in High Reynolds Number Testing.**
Final rept.,
T. V. Vorburger, M. J. McLay, F. E. Scire, D. E. Gilsinn, and C. H. W. Giauque. 1986, 6p
Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center.
Pub. in Jnl. of Aircraft 23, n1 p56-61 Jan 86.

Keywords: *Wind tunnel models, *Surface roughness, Optical measurement, Reynolds number, Reprints, National Transonic Facility.

The paper focuses on stylus and optical techniques for the measurement of surface roughness in wind tunnel models. The stylus instruments provide detailed information, such as surface profiles and area maps, that may then be used either to calculate statistical properties (i.e., the rms surface roughness) or to study individual surface peaks or other features. By contrast, certain optical techniques yield area-averaged statistical properties of the surface roughness directly. Two instruments that use the technique of optical angular scattering are compared. One is a research instrument that has been developed to study the basic scattering phenomena by testing the optical theories and surface models used in inverse calculations of statistical roughness parameters. The second instrument is more compact and is under development as a hand held, on-line device to be used during manufacture of wind tunnel models for the National Transonic Facility at NASA Langley Research Center. The scattering geometries for the two instruments are compared and results from these instruments and the stylus technique are shown for roughness specimens that are typical of the surface finish of wind tunnel models.

# AGRICULTURE & FOOD

## Food Technology

*600,013*
**PB86-202827** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiation Chemistry - Extravaganza or an Integral Component of Radiation Processing of Food.**
Final rept.,
M. G. Simic, M. Dizdaroglu, and E. DeGraff. 1983, 7p
Pub. in Proceedings of the International Meeting of Radiation Processing (4th), Dubrovnik, Yugoslavia, October 4-8, 1982, Radiation Physics and Chemistry 22, n1-2 p233-239 1983.

Keywords: *Food irradiation, Food processing, Radiochemistry, Radiation dose.

The role of radiation chemistry in irradiation processing of foods is discussed in detail. A few examples demonstrating the relevance of radiation chemistry of model systems to the Food Irradiation Technology are given. The importance of irradiation parameters such as dose, dose rate, temperature, atmosphere, physical state and additives in achieving acceptable and high quality of irradiated foods are emphasized. A few examples of radiation-induced free radical reactions in model compounds relevant to foods are also discussed.

# ASTRONOMY & ASTROPHYSICS

## Astrophysics

*600,014*
**N86-32377/1** PC **A03**/MF **A01**
Joint Inst. for Lab. Astrophysics, Boulder, CO.
**Definition and Empirical Structure of the Range of Stellar Chromospheres-Coronae Across the H-R Diagram: Cool Stars.**
J. L. Linsky. 23 Sep 86, 34p NAS 1.26:176863, NASA-CR-176863
Contracts NGL-06-003-057, NAG5-82

Keywords: *Cool stars, *Giant stars, Magnetic flux, *Stellar atmospheres, *Stellar coronas, Stellar magnetic fields, Stellar radiation, A stars, Dwarf stars, Microwaves, Plasmas (Physics), Stellar rotation, Stellar temperature, Supergiant stars, Stellar chromospheres.

Major advances in our understanding of non-radiative heating and other activity in stars cooler than T sub eff = 10,000K has occured in the last few years. This observational evidence is reviewed and the trends that are now becoming apparent are discussed. The evidence for non-radiatively heated outer atmospheric layers (chromospheres, transition regions, and coronae) in dwarf stars cooler than spectral type A7, in F and G giants, pre-main sequence stars, and close binary systems is unambiguous, as is the evidence for chromospheres in the K and M giants and supergiants. The existence of non-radiative heating in the outer layers of the A stars remains undetermined despite repeated searches at all wavelengths. Two important trends in the data are the decrease in plasma emission measure with age on the main sequence and decreasing rotational velocity. Variability and atmospheric inhomogeneity are commonly seen, and there is considerable evidence that magnetic fields define the geometry and control the energy balance in the outer atmospheric layers. In addition, the microwave observations imply that non-thermal electrons are confined in coronal magnetic flux tubes in at least the cool dwarfs and RS CVn systems. The chromospheres in the K and M giants and supergiants are geometrically extended, as are the coronae in the RS CVn systems and probably also in other stars.

*600,015*
**PB86-160116** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**HR Diagram for Normal Radio Stars.**
Final rept.,
D. M. Gibson. 1985, 6p
Pub. in Proceedings of the Radio Stars Workshop, Boulder, CO., June 1984, p213-218 1985.

Keywords: *Radio sources(Astronomy), Binary stars, *Radio stars, Hertzsprung-Russel diagram, Early stars, Late stars, Flare stars, Supergiant stars.

It is found that nonthermal radio emission is associated with stars in very specific locations on the HR diagram. The four classes of objects are typified by early-type mass-loss stars (05/WR), late-type giants and supergiants (M2II), subgiant K-stars (KO IV-III), and flare stars (dMe). The members of each class exhibit about the same maximum radio luminosities, log (L(R)/L(bol)), and flaring timescales, spectra, and polarizations. Membership in a binary system is not found to be a necessary condition for detectable nonthermal emission.

*600,016*
**PB86-161056** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Nonthermal Radio Emission and the HR Diagram.**
Final rept.,
D. M. Gibson. 1985, 5p
Pub. in Proceedings of the NASA (National Aeronautics and Space Administration) Conference on the Origin of Non-Radiative Heating/Momentum in Hot Stars, Greenbelt, MD., June 5-7, 1984, p70-74 1985.

Keywords: *Radio sources(Astronomy), Binary stars, *Radio stars, Hertzsprung-Russel diagram, Early stars, Late stars, Flare stars.

To date, 77 normal stellar objects have been detected and identified as nonthermal radio sources. They are found in four locations on the HR diagram: the 05/WR region, the M2 II region, the KO IV region, and the dM region.

*600,017*
**PB86-162062** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Evidence for Non-Radiative Activity in Stars with T(sub eff) < 10,000K.**
Final rept.,
J. L. Linsky. 1985, 23p
Contract NAG5-82
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of the NASA (National Aeronautics and Space Administration) Conference on the Origin of Nonradiative Heating/Momentum in Hot Stars, Goddard Space Flight Center, Greenbelt, MD., June 5-7, 1984, p24-46 1985.

Keywords: *Stars, Ultraviolet spectra, Radio astronomy, Reviews, Stellar chromospheres, Stellar coronas, Cosmic x-ray sources.

Major advances in the acquisition of evidence for and the understanding of nonradiative heating and other activity in stars cooler than T(eff) = 10,000 K has occurred in the last few years, primarily as a result of the IUE and Einstein spacecraft and the VLA microwave facility. In the paper the author critically reviews the evidence, and comments on the trends that are now becoming apparent.

*600,018*
**PB86-162096** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

## ASTRONOMY & ASTROPHYSICS

### Astrophysics

**Observations of Interstellar C2 toward Three Heavily Reddened Stars.**
Final rept.,
B. L. Lutz, and R. M. Crutcher. 1983, 45p
Grants NSF-AST81-14887, NSF-AST78-20131
Sponsored by National Science Foundation, Washington, DC.
Pub. in Astrophysical Jnl. 271, pL101-L105, 15 Aug 83.

Keywords: *Interstellar matter, *Carbon, Molecules, Abundance, Reprints.

Observations have been made of the 2-0 band of the Phillips system of interstellar C2 toward the heavily obscured early-type stars VI Cygni No. 12, HD 29647, and BD +66 deg 1675. The first direct proof that the rotational excitation temperatures of interstellar C2 are nonthermal was obtained. Toward VI Cygni No. 12, the rotational distribution cannot be characterized by a single, unique excitation temperature; the distribution is consistent with radiative pumping models. A very strong linear correlation was found between N(C2) and E(B-V), which suggests that the relative abundance of C2 is insensitive to a wide variation in physical conditions.

*600,019*
**PB86-163573** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Radiation Driven Stellar Wind Model Atmosphere for the Wolf-Rayet Binary V 444 Cygni.**
Final rept.,
A. Pauldrach, J. Puls, D. G. Hummer, and R. P. Kudritzki. 1985, 4p
Pub. in Astronomy and Astrophysics 148, pL1-L4 1985.

Keywords: *Stellar atmospheres, Binary stars, Reprints, *Wolf-Rayet stars, Stellar winds.

Using the stellar parameters of the WN5 component of the eclipsing binary V 444 Cygni determined by Cherepashchuk et al. (1984) from multi-color light curves, and employing an improved theory of radiatively-driven stellar winds, the authors have calculated models which yield an extended, supersonically expanding photosphere, with values close to those observed for the photospheric radius, the mass-loss rate and the terminal velocity. The radial distributions of velocity and density are also in close agreement with those obtained by Cherepashchuk et al.

*600,020*
**PB86-189172** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Nonradiative Activity across the H-R Diagram: Which Types of Stars Are Solar-Like.**
Final rept.,
J. L. Linsky. 1985, 30p
Grants NAGS-82, NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Solar Physics 100, p333-362 1985.

Keywords: *Stars, Ultraviolet spectra, X ray spectra, Identifying, Sun, Reprints, Stellar chromospheres, Stellar coronas, Hertzsprung-Russell diagram.

The author concludes that dwarf stars of spectral type G-M and rapidly rotating subgiants and giants of spectral type F-K in spectroscopic binary systems are definitely solar-like. Dwarf stars of spectral type A7-F7 are almost certainly solar-like, and T Tauri and other pre-Main-Sequence stars are probably solar-like. Slowly rotating single giants of spectral type F to early K are also probably solar-like, and the helium-strong hottest Bp stars are interesting candidates for being solar-like. The O and B stars exhibit some aspects of activity but probably have weak fields and are not solar-like. Finally, the A dwarfs and the cool giants and supergiants show no evidence of being solar-like.

*600,021*
**PB86-193174** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Ion-Molecule Reaction Probabilities Near 10 K.**
Final rept.,
J. A. Luine, and G. H. Dunn. 1985, 4p
Contract NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Astrophysical Jnl. 299, pL67-L70, 1 Dec 85.

Keywords: *Interstellar matter, Chemical reactions, Molecules, Ions, Nitrogen, Hydrogen, Ammonia, Cryogenics, Reprints, Ion traps.

Reaction probabilities have been measured near 11 K using an ion trap technique for some processes important for molecule formation in interstellar clouds. Probabilities were determined at 11 K = or < T = or < 20 K for the abstraction processes N(1+) + H2 -> NH(1+) + H and NH3(1+) + H2 -> NH4(1+) + H. New experimental upper limits were determined at 11 K for the radiative association reactions C(1+) + H2 -> CH2(1+) + h(nu) and HCO(1+) + H2 -> H3CO(1+) + h(nu). Reaction rate coefficients were deduced from the probabilities.

*600,022*
**PB86-193216** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Photospheric Magnetic Field of the dM3.5e Flare Star AD Leonis.**
Final rept.,
S. H. Saar, and J. L. Linsky. 1985, 4p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 299, n1 pL47-L50, 1 Dec 85.

Keywords: Infrared spectra, Reprints, *Flare stars, *Stellar magnetic fields, AD Leo star.

A high-resolution infrared spectrum of the dM3.5e flare star AD Leo, obtained with the Kitt Peak 4 m Fourier Transform Spectrometer, clearly shows the presence of strong magnetic fields. This is the first detection of photospheric fields on a dMe star.

*600,023*
**PB86-200995** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Optical Region Elemental Abundance Analyses of B and A Stars 4. Re-Evaluation with New Critically Compiled Fe II Oscillator Strengths and Improved Estimates of the Damping Constants.**
Final rept.,
S. J. Adelman, and J. R. Fuhr. 1985, 5p
Pub. in Astronomy and Astrophysics 152, p434-438 1985.

Keywords: *Stars, Abundance, Damping, Iron, Reprints, Oscillator strengths.

A new critical compilation of Fen f-values has recently been completed by Martin et al. To see how these values affect the derived stellar abundances both directly in changing the values of log Fe/H for individual lines and through the determination of the microturbulent velocities, the data for eleven (six normal and 5 slightly peculiar) sharp-lined B and A stars have been reanalyzed. At the same time, the choice of line damping constants has been investigated, especially for Fe I and Fe II lines.

*600,024*
**PB86-204583** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision,**
F. J. Lovas. c1986, 51p
Included in Jnl. of Physical and Chemical Reference Data, v15 n1 p251-303 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Microwave spectra, Radio astronomy, Hyperfine structure, *Interstellar gas, *Molecular clouds.

Accurate transition frequencies for the transitions of the molecular species detected in interstellar clouds are presented. These are recommended for reference in future astronomical observations in the radio and microwave regions. The transition frequencies have been selected through critical examination and analysis of the spectroscopic data in the literature. The species identity, quantum number labels, and probable error limits (2 o sigma) are presented for each transition. Representative line antenna temperatures are also given for a typical source as a convenience to users. References are cited to both the astronomical and laboratory literature.

*600,025*
**PB86-212800** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Radio Continuum Emission from Winds, Chromospheres and Coronae of Cool Giants and Supergiants.**
Final rept.,
S. A. Drake, and J. L. Linsky. Mar 86, 19p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astronomical Jnl. 91, n3 p602-620 Mar 86.

Keywords: *Giant stars, *Radio sources(Astronomy), Reprints, *Supergiant stars, Stellar chromospheres, Stellar coronas, Stellar winds, Late stars.

In the paper the authors present the results of a sensitive VLA radio continuum survey at 6 cm of 39 of the nearest, single cool giants and supergiants with spectral types in the range G0-M5. The findings are discussed in the context of the various mechanisms that might be producing radio emission in these cool stars.

*600,026*
**PB86-212826** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Simple Explanation for the Linsky-Haisch Boundary Line for Transition Layers.**
Final rept.,
E. Bohm-Vitense. 1986, 5p
Pub. in Astrophysical Jnl. 301, p297-301, 1 Feb 86.

Keywords: Reprints, *Stellar chromospheres, *Stellar coronas, Transition layers.

It was found that for stars with low gravitational acceleration, transition layers between chromosphere and corona cannot form, because the chromospheres are so extended that the mechanical energy flux decreases faster than the square of the electron density. There is not enough flux left to lead to a steep temperature increase in the transition layer and corona. If the dissipation length lambda for the mechanical energy flux is the same for all stars, the boundary line for transition layers would be expected to coincide with a line of g=const in the H-R diagram. The numerical value for the g depends on the dissipation length. A comparison with the observed boundary line shows that the dissipation length is not the same for all stars but increases roughly as to (Teff/G)to the 0.93 power.

*600,027*
**PB86-212883** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**6 Centimeter Radio Survey of Short-Period Active Binary Stars.**
Final rept.,
S. A. Drake, T. Simon, and J. L. Linsky. May 86, 4p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astronomical Jnl. 91, n5 p1229-1232 May 86.

Keywords: *Binary stars, Radio sources(Astronomy), Reprints, Stellar coronas.

The authors have observed 13 binaries with periods in the range of 0.2 -2.0 days at 6 cm wavelength with the VLA. Eight out of these 13 systems were detected, of which seven are RS Canum Venaticorum systems and one is an Algol system, with observed fluxes in the range of 0.3-5.0 mJy. They briefly discuss the individual characteristics of the detected sources. As a group, relative to active binaries of longer orbital periods, the short-period active binaries have a slightly lower mean radio luminosity. There is also a clear correlation of high radio luminosity with high x-ray luminosity evident in these short-period systems, although the authors cannot determine a functional dependence from noncontemporary data.

*600,028*
**PB86-228640** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Cepheid Mass Problem and Cepheid Binaries.**
Final rept.,
E. Bohm-Vitense. Apr 86, 11p
Grant NSG-5398
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 303, p262-272, 1 Apr 86.

Keywords: Stellar evolution, Binary stars, Mass, Reprints, *Cepheid variable stars.

Existing mass determinations for Cepheids with different periods are examined. Wesselink masses are independent of the adopted distance scale. For short periods (<6 days) they follow the sequence of evolutionary masses. For periods longer than 10 days they are lower by up to a factor of 2. The lower mass branch joins up with the bump masses. The new pulsational masses agree with the Wesselink masses for periods longer than 6 days. Cepheid masses determined by means of their giant companions also agree with the Wesselink masses and the new pulsational masses. While the error bars are large, the derived dynamical masses determined for S Mus and V636 Sco also agree with the low Wesselink and giant companion masses.

*600,029*
**PB86-228665** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**SN 1985f: Death of a Wolf-Rayet Star.**
Final rept.,
M. C. Begelman, and C. L. Sarazin. Mar 86, 4p
Grant NSF-AST83-51997
Sponsored by National Science Foundation, Washington, DC.
Pub. in Astrophysical Jnl. 302, n2 pL59-L62, 15 Mar 86.

Keywords: *Supernoval, Reprints, *Wolf-Rayet stars, Supernova remnants, Cobalt 56, Nucleosynthesis.

From an analysis of the optical spectrum of SN 1985f, the authors show that the supernova ejecta contain about or > 5 solar masses of oxygen and very little hydrogen. They suggest that the explosion resulted from the pair instability supernova of a about 50 solar masses WO Wolf-Rayet star. The optical luminosity of the supernova is powered by the radioactive decay of (56)Co synthesized in the explosion. From the rate of decay of the optical emission, the authors estimate that the explosion occurred about 350 days before it was discovered in 1985 February.

*600,030*
**PB86-229275** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**IUE Observations of Interstellar Hydrogen and Deuterium toward Alpha Centauri B.**
Final rept.,
W. B. Landsman, J. Murthy, R. C. Henry, H. W. Moos, and J. L. Linsky. 1986, 6p
Grants NAG5-82, NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 303, p791-796, 15 Apr 86.

Keywords: *Interstellar matter, Hydrogen, Deuterium, Ultraviolet spectra, Reprints, Alpha Centauri B star, IUE.

A profile is presented of the Ly alpha emission line of alpha Cen B (K1V,d=1.3 pc), obtained by addition of two IUE small-aperture, high-dispersion images.

*600,031*
**PB86-229283** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Outer Atmosphere of Procyon (alpha CMi F5IV-V): Evidence of Supergranulation or Active Regions.**
Final rept.,
C. Jordan, A. Brown, F. M. Walter, and J. L. Linsky. 1986, 12p
Grant NAG8-477
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Monthly Notices of the Royal Astronomical Society 218, p465-476 1986.

Keywords: Ultraviolet spectra, X rays, Granulation, Reprints, *Procyon star, Stellar chromospheres, Stellar coronas, X ray astronomy, Stellar activity.

Observations made with the Einstein X-ray observatory and EXOSAT have shown Procyon(alpha CMi) to have a measurable X-ray flux. The flux observed is similar to the upper limits previously reported. The authors discuss the interpretation of the X-ray data in the context of models made previously by Brown & Jordan based on spectra obtained with the IUE satellite.

*600,032*
**PB86-229291** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Ultraviolet, Optical, Infrared, and Microwave Observations of HR 5110.**
Final rept.,
I. R. Little-Marenin, T. Simon, T. R. Ayres, N. L. Cohen, and P. A. Feldman. 1986, 11p
Grant NAG5-82
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 303, n2 p780-790, 15 Apr 86.

Keywords: *Binary stars, Ultraviolet spectra, Reprints, Late stars, Algol system, IUE.

HR 5110 is a close binary system which is viewed nearly pole-on (i=13 deg). A comparison of the characteristics of Algol and RS CVn systems to those of HR 5110 shows that HR 5110 can also be considered an Algol system. Because the primary star is relatively cool (F21V) and there is no apparent emission from an accretion disk, the authors are able to detect in IUE spectra the emission of an active chromosphere and transition region of the cooler (K0 IV) secondary. HR 5110 is important because it is the only known Algol system for which the properties of the secondary star can be studied in detail.

*600,033*
**PB86-230786** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Magnetic Field of the BY Draconis Flare Star EQ Virginis.**
Final rept.,
S. H. Saar, J. L. Linsky, and J. M. Beckers. Mar 86, 8p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 302, n2 p777-784, 15 Mar 86.

Keywords: Reprints, *Flare stars, *Stellar magnetic fields, Late stars, EQ Virginis star.

A new Zeeman analysis procedure, which includes radiative transfer effects and compensation for blends, was applied to high-resolution, high-signal-to-noise line profiles of the BY Draconis-type flare star EQ Vir obtained with the Multiple Mirror Telescope. Using a number of lines with effective Lande g factors ranging from 0.5 to 2.5, and two different analysis methods, the authors found a mean field of 2500 + or - 300 G covering 80% + or - 15% of EQ Vir.

*600,034*
**PB86-230794** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Unravelling the Oldest and Faintest Recovered Nova: CK Vulpeculae (1670).**
Final rept.,
M. M. Shara, A. F. Moffat, and R. F. Webbink. 1985, 15p
Grants NSF-AST79-21073, NSF-AST80-18859
Sponsored by National Science Foundation, Washington, DC.
Pub. in Astrophysical Jnl. 294, n1 p271-285 1985.

Keywords: *Binary stars, *Novae, Variable stars, Nebulae, Reprints, CK vulpeculae star.

A narrow-band H(alpha) + (N II) CCD image of the field of Nova CK Vul (1670) shows nebulosity with a morphology (suggestive of equatorial ejection) with several bright subcondensations, and a central star. The net H(alpha) image also reveals a faint jet leading to an H(alpha)-bright knot, suggestive of polar ejection.

*600,035*
**PB87-109716** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Molecular Thermal Emission and Its Relationship to Circumstellar Absorption, Stellar Absorption, and Stellar Emission in Red Variables.**
Final rept.,
G. Wallerstein. 1979, 13p
Pub. in Changing Trends in Variable Star Research IUE Colloq. 46, p177-189 1979.

Keywords: Absorption, Stars, Carbon monoxide, Shock waves, Silicon oxides, *Thermal emission, Long period variables, Chi Cygni star, T cepheid star, Mass loss, Stellar mass ejection.

Radial velocity data obtained from thermal SiO and CO as well as various optical features such as photospheric absorption lines, circumstellar features, and shock excited emission lines are assembled. Three types of stars: long period variables, supergiant M stars and semi-regular stars of late spectral type are included. The data are discussed to establish the motion of each layer with respect to the center of the star. For two stars, Chi Cygni and T Cepheid the data are discussed in considerable detail on the basis of spectrograms of very high depression.

*600,036*
**PB87-109724** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Bright Pre-Main Sequence Variable HR 5999.**
Final rept.,
P. S. The, A. Brown, C. Catala, V. Doazan, and F. L. Linsky. 1985, 19p
Pub. in Irish Astronomical Jnl. 17, n2 p79-97 1985.

Keywords: *Variable stars, Reprints, *HR 5999 star, Stellar winds, Stellar chromospheres.

The bright and variable Herbig A7e star HR 5999 (V = 6.8 - 8.0) provides an excellent opportunity to make a detailed study of the properties and behavior of a massive (3 M sub o) solar masses star in the quasi-hydrostatic equilibrium phase of its contraction towards the main sequence. Because of the irregular variability of the star, it is necessary to make coordinated (if possible simultaneous) observations in a wide range of wavelengths in order to delineate the relationship between the various observable quantities of its atmosphere (coulors, emission-line fluxes, wind velocities, etc.) before a dynamical model of the extended atmosphere can be developed. Recently a group of observers joined efforts to make coordinated EXOSAT, IUE and ground-based observations of HR 5999. The observations took place around 11 September 1983. After the observations were reduced, this group met on 7 May 1984 in Amsterdam to discuss these and previous observations. A summary of that meeting is presented.

*600,037*
**PB87-111084** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Stellar Chromospheres, Coronae, and Winds: Present Status and Implications for Solar Astrophysics.**
Final rept.,
J. L. Linsky. 1981, 11p
Contract NAG5-82, Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of Workshop on Precision Doppler Velocity Measurements in Astronomy Solar Instrumentation--What's Next, Sunspot, New Mexico, October 14-17, 1980, p180-190 1981.

Keywords: Chromosphere, Solar corona, Solar wind, *Stellar chromospheres, *Stellar coronas, *Stellar winds, Early stars, Late stars, IUE, HEAO 2.

Some of the important new results that are rapidly emerging from studies with the IUE and Einstein Observatories concerning the existence and properties of stellar chromospheres, coronae, and winds are reviewed, briefly. These results are radically altering our understanding of the outer atmospheres of late-type and early-type stars. They are also raising fundamental questions that can only be answered by new high resolution studies of the Sun. In a sense our vigorous pursuit of the solar stellar connection is about to complete a full circle in which studies of solar phenomena in stars have led to the posing of fundamental questions in astrophysics that require renewed studies of the Sun, but from a stellar perspective. In the paper the author lists a number of these fundamental questions for which well conceived Solar Optical Telescope (SOT) and ground-based observing programs can begin to provide answers.

*600,038*
**PB87-128211** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

## Astrophysics

**Observations of Interstellar HI toward Nearby Late-Type Stars.**
Final rept.,
W. B. Landsman, R. C. Henry, H. W. Moos, and J. L. Linsky. 1984, 4p
Pub. in National Aeronautics and Space Administration Conference Publication, v2345 p60-63 1984.

Keywords: *Interstellar matter, Ultraviolet spectra, OAO 3, IUE.

High-dispersion Copernicus and IUE observations of chromospheric Ly alpha emission are used to study the distribution of HI in the local interstellar medium. Interstellar parameters are derived toward 3 stars within 5 pc of the sun, and upper limits are given for the Ly alpha flux from 9 other stars within 10 pc.

*600,039*
**PB87-128237** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**IUE (International Ultraviolet Explorer) High-Dispersion Cool-Star Atlas.**
Final rept.,
T. R. Ayres, E. W. Brugel, J. L. Linsky, A. Brown, and K. G. Carpenter. 1986, 3p
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Sante Fe, NM., October 16-18, 1985, p106-108 1986.

Keywords: Ultraviolet spectra, Atlases, *Cool stars, Late stars, Stellar chromospheres, IUE.

The authors are planning to compile a spectral atlas based on high-dispersion images of representative late-type stars recorded by the International Ultraviolet Explorer. They solicit advice from the ultraviolet community concerning how best to present the spectral material.

*600,040*
**PB87-128245** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Precise Measurements of Radial Velocities of Far-Ultraviolet Emission Lines in Stars of Late Spectral Type.**
Progress rept.,
T. Ayres, O. Engvold, E. Jensen, and J. L. Linsky. 1986, 3p
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Santa Fe, NM., October 16-18, 1985, p94-96 1986.

Keywords: Ultraviolet spectra, Far ultraviolet radiation, Emission spectra, *beta Draconis star, *Supergiant stars, Late stars, Stellar chromospheres, Radial velocity, IUE.

Recent high-dispersion, far-ultraviolet IUE spectra of the G-type supergiant beta Draconis contain evidence for organized, persistent downflows of gas, apparently confined to a high-density component of the stellar transition zone.

*600,041*
**PB87-128252** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**What Stellar or Solar Radio Observations Teach Us about the Sun or Stars.**
Final rept.,
D. M. Gibson. 1986, 15p
Pub. in Proceedings of INDO/US Workshop on Solar Terrestrial Physics (2nd), New Delhi (India), January 30-February 3, 1984, p43-57 1986.

Keywords: *Solar radio emission, *Solar flares, Solar corona, Extraterrestrial radio waves, *Stellar flares, Stellar coronae, Stellar radiation.

Stellar analogs of solar microwave emissions are but one aspect of the solar stellar connection (SSC). In the paper, the author summarizes these observations, and shows how application of the SSC allows us to obtain fundamental insights into two important aspects of solar and stellar activity-flares and activity cycles.

*600,042*
**PB87-128260** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Advanced X-ray Astronomical Facility (AXAF): A Powerful New Tool for Probing Stellar Coronae.**
Final rept.,
J. L. Linsky, and M. C. Weisskopf. 1986, 3p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Sante Fe, NM., October 16-18, 1985, p250-252 1986.

Keywords: X ray spectra, *X ray astronomical facility, *X ray astronomy, *Stellar coronae.

AXAF, the next major step in NASA's program for X-ray astronomy, is presently in its Phase B definition and design phase and could be launched as early as 1993. The AXAF will be a long duration (> 15 years) national observatory with a majority of the observing time set aside for guest investigators. AXAF will have a grazing incidence telescope consisting of six nested Wolter type I paraboloid-hyperboloid mirror pairs ranging in diameter from 0.6 to 1.2 m, and a complement of powerful imaging and spectroscopic instruments. The telescope will have an angular resolution of 0.5 arcsecond, collecting area of 1700 sq cm, and significant energy response up to 10 keV. These characteristics and the modern instruments result in AXAF being a far more powerful observatory than HEAO-2 (Einstein) for probing stellar coronae.

*600,043*
**PB87-128740** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Transition Regions of Warm Stars.**
Final rept.,
F. M. Walter, and J. L. Linsky. 1986, 3p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Santa Fe, NM., October 16-18, 1985, p50-52 1986.

Keywords: *Stars, Stellar chromospheres, Stellar coronae, Stellar magnetic fields.

There is a fundamental difference between the hot and cool stars. The former have convective envelopes, which manifest themselves in solar-like, magnetically driven activity, whereas the latter winds have radiatively-driven winds and exhibit different kinds of nonthermal activity. The transition occurs in the late-A or early F dwarfs. Theoretical considerations imply that the convective zone becomes thin in the early F dwarfs, and should effectively disappear by B-V = 0.30. Observations of stellar activity near this color should permit verification of the disappearance of the convective zone, as the convectively driven stellar activity might be expected to disappear as well. Furthermore, measurements of parameters for this activity may yield greater understanding of the convective zone and stellar dynamos.

*600,044*
**PB87-128757** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Time Variability of Magnetic Fields on Epsilon Eridani.**
Final rept.,
S. H. Saar, J. L. Linsky, and D. K. Duncan. 1986, 3p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Santa Fe, NM., October 16-18, 1985, p275-277 1986.

Keywords: *Stars, *Stellar magnetic fields, Epsilon Eridani star, Time dependence.

Since the first detections of magnatic fields on late-type dwarfs, the derived magnetic parameters have almost entirely been 'snapshots' of a given star's magnetic activity. Little is known about the distribution of fields with phase or their time evolution on any star other than the Sun. The authors have begun a synoptic program of stellar magnetic field measurements using the NSO McMath echelle/Reticon system to search for both rotational modulation of active regions and the growth and decay of magnetic areas with time. Both the area filling factor of active regions and the mean magnetic field in these regions are measured. The authors present some initial results from the program.

*600,045*
**PB87-128765** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Further Observations of Magnetic Fields on Active Dwarf Stars.**
Final rept.,
S. H. Saar, and J. L. Linsky. 1986, 3p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Santa Fe, NM., October 16-18, 1985, p278-280 1986.

Keywords: *Dwarf stars, *Stellar magnetic fields.

In previous studies, about 20 detections of field strengths (B) and surface area coverages (f) on some 35 stars have been made, using techniques pioneered by Robinson and Marcy. Surface averaged fields for the active G and K stars are typically about 700 G. Recent discoveries of fields on very chromospherically active flare and BY Draconis stars, however, reveal that these stars generate substantially more magnetic flux (<B>approx=2-3000 G). Extending this work, the authors present here photospheric magnetic field measurements for five more very active dwarfs.

*600,046*
**PB87-128773** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**HR 5110: An Algol System with RS CVn Characteristics.**
Final rept.,
I. R. Little-Marenin, J. L. Linsky, and T. Simon. 1986, 3p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun (4th), Santa Fe, NM., October 16-18, 1985, p247-249 1986.

Keywords: *Binary stars, Ultraviolet spectra, IUE.

HR 5110 (HD 118216=BH CVn) is a close binary system which is viewed nearly pole-on (i=13 degrees). A comparison of the characteristics of Algol and RS CVn systems to those of HR 5110 shows that HR 5110 can also be considered an Algol system. Because the primary star is relatively cool (F2 IV) and there is no apparent emission from an accretion disk, the authors are able to detect in IUE spectra the emission of an active chromosphere and transition region of the cooler secondary. HR 5110 is the only known Algol system for which the properties of the secondary star can be studied in detail.

*600,047*
**PB87-134185** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Intrinsic Parameters of Hot Blue Stars.**
Final rept.,
R. P. Kudritzki, and D. G. Hummer. 1986, 16p
Pub. in Luminous Stars and Associations in Galaxies, p3-18 1986.

Keywords: Stellar atmospheres, Galaxies, Reprints, *Hot stars, *Blue stars.

Advances in both theoretical understanding and observational capabilities in the past few years have made possible the determination of the effective temperature, surface gravity, and chemical abundance of massive stars with unprecedented accuracy. These data are in turn important for the study of galaxies, as stars are important sources of information concerning the evolutionary state, past and present chemical composition, and distance of the parent galaxy. In addition to this diagnostic role, stars are crucial as sources of light, matter, and metals in the galaxy. Thus an improved understanding of massive stars makes possible a better determination of the physical conditions in a galaxy as well as a deeper understanding of how it functions.

## Cosmic Ray Research

*600,048*
**PB87-115424** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Flux Limit of Cosmic-Ray Magnetic Monopoles from a Multiply Discriminating Superconducting Detector.**
Final rept.,
M. W. Cromar, A. F. Clark, and F. R. Fickett. 1986, 3p
Pub. in Physical Review Letters 56, n24 p2561-2563, 16 Jun 86.

Keywords: *Cosmic rays, Superconductors, Detectors, Reprints, *Magnetic monopoles.

A multiply discriminating, three-loop superconducting monopole detector was operated for 1 yr. During this period 8523 h of data were accumulated. The sensing area averaged over solid angle for trajectories passing through a loop was 178 sq cm. With inclusion of double-coincidence events from trajectories passing through the shield but not through a loop, the total sensing area averaged over solid angle was 1195 sq cm. No candidate monopole events were observed; this leads to an upper limit on the flux of cosmic-ray magnetic monopoles of 5.0 x 10 to the -12th power/sq cm sr s with a 90% confidence level.

# ATMOSPHERIC SCIENCES

## Aeronomy

*600,049*
**PB86-185469** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Auroral Implications of Recent Measurements on O(1S) and O(1D) Formation in the Reaction of N(+) with O2.**
Final rept.,
A. O. Langford, V. M. Bierbaum, and S. R. Leone. 1985, 4p
Contract F49620-83-X-0013
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Planetary and Space Science 33, p1225-1228 1985.

Keywords: *Auroras, Emission spectra, Oxygen, Reprints, Ion-molecule collisions, Nitrogen ions.

Recent flowing afterglow measurements have shown that the reaction of N(1+) with O2 produces 70 + or - 30% of the oxygen atom product as O(singlet D) and <0.1% as O(singlet S). These results indicate that this reaction does not contribute to the auroral green line emission (5577 A), but can account for about 10% of the observed red line (6300 A) auroral emission.

## Dynamic Meteorology

*600,050*
**PB86-169026** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Directional Hurricane Wind Speeds.**
Final rept.,
E. M. Hendrickson, and E. Simiu. Feb 86, 34p NBSIR-86/3317
See also PB81-143224. Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: *Wind velocity, *Hurricanes, *Coasts, Estimating, Wind direction, Statistical analysis, Sites, Nuclear power plants, Wind pressure, Magnetic tapes, Climate.

The report presents a simple procedure for estimating coastline hurricane wind speeds corresponding to any specified set of wind directions and to any specified mean recurrence interval. The procedure uses simulated directional hurricane wind speed data as described in the report Hurrican Wind Speeds in the United States (NBS BSS 124). These data are encoded on magnetic tape for 56 mileposts located along the U.S. Gulf and Atlantic coasts.

*600,051*
**PB86-199932** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Wind Speed Estimation Errors in Hurricane Alicia.**
Final rept.,
R. D. Marshall. 1985, 11p
Pub. in Proceedings of Hurricane Alicia: One Year Later, Galveston, TX., August 16-17, 1984, p70-80 1985.

Keywords: *Wind velocity, *Hurricanes, Boundary layer, Errors, Weather observation, Mathematical models, Tropical cyclones, Structural engineering, Atmospheric boundary layer, *Hurricane Alicia.

The transformation of surface wind speeds observed in Hurricane Alicia to fastest-mile speeds corresponding to standard conditions makes use of representations of the atmospheric boundary layer that are based upon mean wind speeds averaged over a period of approximately 1 hour. Errors involved with estimating fastest-mile wind speeds include observation errors, site characterization errors, and modeling errors. When combined with modeling errors, estimates of fastest-mile speeds can be expected to have a range of error of about + or - 12 percent when derived from strip-chart records, and about + or - 16 percent when derived from hourly observations.

## Meteorological Data Collection, Analysis, & Weather Forecasting

*600,052*
**PB87-140422** PC **A13**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Handbook for the Quality Assurance of Meteorological Measurements.**
Final rept.,
J. K. Taylor, and H. V. Oppermann. Nov 86, 290p NBS/HB-145
Library of Congress catalog card no. 86-600583. Also available from Supt. of Docs. as SN003-003-02774-0.

Keywords: *Meteorological data, *Metrology, Quality assurance, Handbooks, Calibrating, Standards, Precision, Accuracy.

The general concept of quality assurance for metrological measurements is discussed. A number of Good Laboratory Practices (GLPs) and Good Measurement Practices (GMPs) related to metrology are compiled. Twenty recommended Standard Operations Procedures (SOPs) for high-accuracy mass, length, and volumetric calibrations made most frequently by State weights and measures laboratories are included. The statistical techniques useful for evaluating measurement quality are reviewed. Control charts most useful for metrological measurements are discussed.

## Meteorological Instruments & Instrument Platforms

*600,053*
**PB86-245735** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Final Evaluation of a Color Calibrator for a Radar Remote Weather Display System,**
L. G. Porter. Jul 86, 86p NBSIR-86/3403
Sponsored by Federal Aviation Administration, Washington, DC.

Keywords: *Meteorological radar, *Remote sensing, *Color codes, Display systems, Cathode ray tubes, Standardization, Calibration.

The report deals with the development and field testing of an inexpensive color calibrator for the standardization of the Weather Intensity Level (WIL) colors used in the FAA's Radar Remote Weather Display System or RRWDS. The report covers the field validation of the color calibrator and, as an end product, the construction of a tentative look-up table that identifies whether the six WIL colors are within acceptable limits. In addition, the report includes a general review of significant literature on color-coding, since RRWDS color codes weather information. The report presents first-of-its-kind objective data on the effects of ambient room lighting on colors used in a self-luminous display.

## Physical Meteorology

*600,054*
**PB86-200763** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Microwave Spectra of Atmospheric Species.**
Final rept.,
F. J. Lovas. 1985, 13p
Pub. in Proceedings of CMA/NBS Workshop on Atmospheric Spectra, Gaithersburg, MD., November 3-4, 1983, p111 A14-III A26 Jun 85.

Keywords: *Atmospheric composition, Microwave spectroscopy, Molecular structure, *Chlorine nitrate(ClNO3), *Chlorine oxides, *Hypochlorous acid.

The status of microwave spectroscopy as applied to the property of the earth's atmosphere is described. The pertinent microwave literature is reviewed for molecular species present in trace amounts in the atmosphere according to their relative importance. New work on chlorine nitrate, hypochorous acid and chlorine monoxide performed at NBS is presented.

*600,055*
**PB86-200771** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Critically Evaluated Microwave Spectral Data.**
Final rept.,
F. J. Lovas. Jun 85, 8p
Pub. in Proceedings of CMA/NBS Workshop on Atmospheric Spectra, Gaithersburg, MD., November 3-4, 1983, pIV-21-IV-28 Jun 85.

Keywords: *Microwave spectra, *Atmospheric composition, Molecular spectra.

A discussion is presented on the critical evaluation and cataloging of microwave spectra with special attention being given to those molecular species that play a role in the chemistry of the upper atmosphere. Data to be compiled and evaluated are spectral observations, molecular constants, and the sources of the data according to experimental technique.

*600,056*
**PB86-207172** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Review of the Quail Roost II Receptor Model Simulation Exercise.**
Final rept.,
R. W. Gerlach, L. A. Currie, and C. W. Lewis. 1982, 14p
Pub. in Proceedings of Specialty Conference on Receptor Models Applied to Contemporary Pollution Problems, Danvers, MA., October 17-20, 1982, SP48, p96-109.

Keywords: *Atmospheric composition, *Aerosols, *Mathematical models, *Atmospheric models, Computerized simulation, Atmospheric dispersion, Intercomparison.

As a principal component of the Quail Roost II Receptor Model Workshop (March 1982) three sets of ambient aerosol compositional data were generated by computer simulation and distributed to several participants as a preliminary exercise in receptor model intercomparison and validation. The specific objectives of the exercise were: (a) to judge the resolving power and accuracy of alternative source apportionment methods; (b) to judge the meaninfulness of predicted vs. actual uncertainties in source apportionment; and (c) to judge the adequacy of the preliminary synthetic data

set as a standard test bed for defining the performance of candidate methods. Generation of the data sets was accomplished through the use of the RAM dispersion model with real meteorological data, reasonable chemical source profiles for up to 13 source types, and random profile and measurement errors for nineteen elements and one isotopic ratio ((14)C/(12). Geographic placement of the sources and emissions rates were adjusted to yield an interesting level of complexity at the (single) receptor site.

*600,057*
**PB86-240090** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Ultraviolet Cross-Sections of Ozone. 1. The Measurements.**
Final rept.,
A. M. Bass, and R. J. Paur. 1985, 6p
See also PB86-240108.
Pub. in Proceedings of Quadrennial Ozone Symposium, Halkidiki, Greece, September 3-7, 1984, Atmospheric Ozone, p606-610 1985.

Keywords: *Ozone, Absorption cross sections, Ultraviolet absorbers, Atmospheric attenuation, Temperature dependence, Atmospheric transmissivity.

Absorption cross-sections of ozone have been measured over the range 230 nm to 350 nm, and for temperatures 200K to 300K, with improved photometric accuracy and spectral resolution. These measurements are referred to the cross-section at the 253.65 nm mercury line, 1147 x 10 to the -20th power sq cm, and show an internal consistency of + or -1%.

*600,058*
**PB86-240108** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Ultraviolet Cross-Section of Ozone. 2. Results and Temperature Dependence.**
Final rept.,
R. J. Paur, and A. M. Bass. 1985, 6p
See also PB86-240090.
Pub. in Proceedings of Quadrennial Ozone Symposium, Halkidiki, Greece, September 3-7, 1984, Atmospheric Ozone, p611-616 1985.

Keywords: *Ozone, Absorption cross sections, Ultraviolet absorbers, Atmospheric attenuation, Temperature dependence, Atmospheric transmissivity.

Tables of ozone absorption cross-section in the ultraviolet have been prepared for intervals of 0.05 nm over the range 245 to 340 nm. At each wavelength entry in the table a set of coefficients has been derived that permits the cross-section to be computed as a function of temperature, between 200K and 300K, with an accuracy of 1%.

# BIOMEDICAL TECHNOLOGY & HUMAN FACTORS ENGINEERING

## Biomedical Instrumentation & Bioengineering

*600,059*
**PB86-160561** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**NBS (National Bureau of Standards) Hearing Aid Test Procedures and Test Data.**
Final rept.,
E. D. Burnett, M. T. Tarica, and P. A. Jurgens. 1983, 355p
Sponsored by Veterans Administration, Washington, DC.
Pub. in Veterans Administration Handbook of Hearing Aid Measurement, p7-361 1983.

Keywords: *Medical equipment, Responses, Tests, Procedures, Reprints, *Hearing aids, Veterans Administration, National Bureau of Standards.

The methods used by NBS for testing hearing aids for the Veterans Administration are described. Several possible methods of measuring the acoustic response of hearing aids are discussed, with emphasis on the measurement of the insertion response, which is the method used by NBS. The measurement method for determining the saturation sound pressure level, gain, harmonic distortion, equivalent input noise level, frequency response, telephone coil sensitivity, and characteristics of special-purpose hearing aids are discussed.

*600,060*
**PB86-230513** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Chemically Modified Electrode Sensors.**
Final rept.,
R. A. Durst, and E. A. Blubaugh. Oct 85, 11p
Pub. in ACS Symposium Series No. 309, p245-255, 1 Oct 85.

Keywords: Chemical analysis, Electrodes, Fabrication, Bioinstrumentation, Reprints, *Chemically modified electrodes.

The review gives a brief summary of the types of chemically modified electrodes, their fabrication, and some examples of their uses. One especially promising area of application is that of selective chemical analysis. In general, the approach used is to attach to the electrode surface electrochemically reactive molecules which have electrocatalytic activity toward specific substrates or analytes. In addition, the incorporation of biochemical systems should greatly extend the usefulness of these devices for analytical purposes.

*600,061*
**PB86-231586** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Dependence of Curing Time, Peak Temperature, and Mechanical Properties on the Composition of Bone Cement.**
Final rept.,
G. M. Brauer, D. R. Steinberger, and J. W. Stansbury. 1986, 14p
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Jnl. of Biomedical Materials Research 20, p839-852 1986.

Keywords: *Bone cements, *Curing, *Composite materials, Temperature, Mechanical properties, Composition, Reprints.

Commercial bone cements usually contain hydroquinone as the polymerization inhibitor and N,N-dimethyl-p-toluidine as the accelerator in the benzoyl peroxide-initiated redox polymerization. The former compounds have certain shortcomings in their biocompatibility profile. Measurements of the setting times, polymerization exotherms, and postpolymerization strengths of the cured monomer-polymer compositions show that the hydroquinone can be replaced by food grade di-tert-butyl-p-cresol(BHT). The more reactive 4-N,N-(dimethylamino)phenethanol can replace 4-N,N-dimethyl-p-toluidine, yielding cements with shorter setting times and increased strengths. Excessive heat liberated on polymerization can be reduced by partial substitution of higher-molecular-weight methacrylates, e.g., dicyclopentenyloxyethyl methacrylate for methyl methacrylate, but there is a decrease in strength of the resulting polymer.

*600,062*
**PB86-241882** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
**Dental Base-Metal Casting Alloys: Physical Metallurgy.**
Final rept.,
J. A. Tesk, and R. M. Waterstrat. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p1056-1060 1986.

Keywords: *Dental materials, Cobalt alloys, Nickel alloys, Stainless steels, Titanium alloys, Reprints, *Casting alloy.

Composition, properties and microstructure of nonprecious dental casting alloys are reviewed. Relevance to needs for clinical performance is discussed and clinical applications for each class of alloy is presented. Alloy systems include Cobalt-Chromium-Molybdenum, Nickel-Chromium, Ferritic and Austenitic Stainless Steels and Titanium Alloys.

## Bionics & Artificial Intelligence

*600,063*
**PB86-238839** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Structure for Generation and Control of Intelligent Behavior.**
Final rept.,
J. S. Albus. 1983, 4p
Pub. in Proceedings of Institute of Electrical and Electronics Engineers International Conference on Computer Design: VLSI in Computers, Port Chester, NY., October 31-November 3, 1983, p25-28.

Keywords: *Planning, Intelligence, Behavior, Objectives, *Artificial intelligence, *learning machines, Goals, Computer architecture.

A hierarchical architecture which has the ability to generate and control intelligent behavior is presented. Three parallel cross-coupled hierarchies are proposed of (1) a task or goal decomposition hierarchy, (2) a sensory processing hierarchy, and (3) a world modeling hierarchy. The upper levels of these hierarchies have the ability to select goals, evaluate results, and generate plans. Intelligence is defined to be the set of computing mechanisms that enable an organism or a machine: (1) to select good goals, and (2) to act in a manner which tends to optimize the probability of success in achieving the selected goals.

*600,064*
**PB87-129037** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Survey of Current Robot Metrology Methods.**
Final rept.,
K. Lau, and R. J. Hocken. 1984, 4p
Pub. in CIRP Annals 33, n2 p485-488 1984.

Keywords: *Robots, Metrology, Instruments, Reproducibility, Kinematics, Dynamics, Accuracy, Tests, Laboratories, Research projects.

In response to industrial needs, performance measures for robots are being developed in laboratories around the world. Although as yet no universally accepted tests for robots have been adopted, researchers have developed or are developing procedures in instrumentation for examining repeatability, kinematics, dynamics, and positioning accuracy of industrial robots.

## Human Factors Engineering

*600,065*
**AD-P002 927/2** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Washington, DC.
**Ergonomic Data Base for Physical Security,**
P. C. Goodman. 1 Jun 81, 8p
Pub. in Proceedings of the Symposium on the Role of Behavioral Science in Physical Security (5th Annual) Held at Gaithersburg, MD., June 11-12, 1980, AD-A138 882, p141-148.

Keywords: *Ergonomics, *Area security, *Data bases, Man machine systems, Human factors engineering, Warning systems, Intrusion detection, Behavioral science, Component Reports, Physical security.

The National Bureau of Standards has been exploring the possibility of developing an ergonomics data system since 1976. We summarize some of our preliminary findings and outline our future plans to extend this work to benefit the multidisciplinary field of physical security.

## Life Support Systems

*600,066*

**PB87-140299** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Application of Smoke Detector Technology to Quantitative Respirator Fit Test Methodology.**
Final rept.,
G. W. Mulholland, R. Bukowski, B. Y. H. Liu, and V. Szymanski. Nov 86, 63p NBSIR-86/3481
Prepared in cooperation with Minnesota Univ., Minneapolis. Particle Technology Lab. Sponsored by Occupational Safety and Health Administration, Washington, DC.

Keywords: *Respirators, Test methods, Measurement, Design, *Smoke detectors, Human factors engineering.

A quantitative respirator fit test apparatus was developed based on using a light-scattering type smoke detector for the sensing element and a clinical nebulizer for the aerosol source. The performance of three smoke detectors and nine clinical nebulizers considered for use in the final system are reported. Key design features of the apparatus include the generation of a corn oil aerosol concentration of 500 mg/m3 at a flow rate of 50 l/min and LED display for protection factors of 25, 50, 125, and 450. The total cost of the component parts for the apparatus is less than $300. The apparatus is designed to meet the need for a low cost, easy to use instrument for quantitatively monitoring a respirator's fit to a worker's face.

## Prosthetics & Mechanical Organs

*600,067*

**PB86-201407** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Mechanical Properties and Structure of Ti-6A1-4V with Graded-Porosity Coatings Applied by Plasma Spraying for Use in Orthopedic Implants.**
Final rept.,
H. Hahn, P. J. Lare, R. H. Rowe, A. C. Fraker, and F. Ordway. 1985, 13p
Pub. in Proceedings of the Corrosion and Degradation of Implant Materials Symposium (2nd), Louisville, KY., May 9-10, 1983, ASTM (American Society for Testing and Materials) Spec. Tech. Pub. 859, p179-191 1985.

Keywords: Titanium alloys, Aluminum containing alloys, Vanadium containing alloys, Coatings, Mechanical properties, Corrosion fatigue, *Surgical implants, Titanium alloy 6 Al 4V.

The object of the work was to determine mechanical properties of implants with graded porous coatings without reference to the properties of the ingrown bone. Optimum strength of a bone/implant interface consisting of porous metal and ingrown bone requires a gradation from base metal to the original bone. The composite metal-bone interface can be obtained by applying a metal coating of graded porosity, varying from near zero at the substrate surface to more than 50% at the outermost layer on the original implant. Graded porous coatings of titanium or Ti-6Al-4V were obtained by plasma spraying of selected particle size fractions in three layers of successively decreasing density the top coat being made with 300 to 850 pm powder. Tensile and shear strengths of the coatings were determined by cementing coated samples face to face with an adhesive resin to simulate ingrown bone. Data from these tests are given. Shear strength values ranged from 5.6 to 9.9 MPa (815 to 1430 psi) and tensile strength values were 5.1 to 25. 5 MPa (745 to 3700 psi). Failure occurred within the porous coating and not at the interface between the substrate and the coating. Corrosion fatigue tests in Hanks' solution at 37 deg. C (98.6 deg. F) and a pH of 7.4, with a cyclic, fully reversed, peak torsional shear strain of plus or minus 0.01, gave lifetimes comparable to or better than those reported for mill-annealed Ti-6Al-4V, except for the samples that had been smtered.

# BUILDING INDUSTRY TECHNOLOGY

## Architectural Design & Environmental Engineering

*600,068*

**AD-A154 174/7** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Airborne Sound Transmission Loss Characteristics of Wood-Frame Construction.**
Forest Service general technical rept.,
F. F.Rudder. Mar 85, 30p Rept no. FSGTR-FPL-43

Keywords: *Sound transmission, *Transmission loss, *Wood, Airborne, Buildings, Construction materials, Data bases, Doors, Laboratory procedures, Measurement, Methodology, Numerical methods and procedures, Predictions, Sound transmission, Transmission loss, Walls, Acoustic absorption, Acoustic materials, Frames, Theory, Acoustic properties, Floors, Ceiling, Wood frame construction.

This report summarizes the available data on the airborne sound transmission loss properties of wood-frame construction and evaluates the methods for predicting the airborne sound transmission loss. The first part of the report comprises a summary of sound transmission loss data for wood-frame interior walls and floor-ceiling construction. Data bases describing the sound transmission loss characteristics of other building components, such as windows and doors, are discussed. The second part of the report presents the prediction of the sound transmission loss of wood-frame construction. Appropriate calculation methods are described both for single-panel and for double-panel construction with sound absorption material in the cavity. With available methods, single-panel construction and double-panel construction with the panels connected by studs may be adequately characterized. Technical appendices are included that summarize laboratory measurements, compare measurement with theory, describe details of the prediction methods, and present sound transmission loss data for common building materials.

*600,069*

**PB86-165438** PC **A07**/MF **A01**
West Virginia Univ., Morgantown. Dept. of Civil Engineering.
**Convective Heat Loss from Windows: A Review of the Literature,**
D. D. Gray. Feb 86, 127p NBS/GCR-86/504
Contract DE-AC02-83CH10093
Prepared in cooperation with American Society for Engineering Education, Washington, DC. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and Department of Energy, Washington, DC.

Keywords: *Windows, *Heat loss, Convection, Tests, U-values.

It is necessary to be able to calculate heat loss through fenestration systems such as windows, patio doors, and skylights, in order to size building equipment for peak loads and to estimate annual energy costs for buildings. One of the most important factors that influences thermal performance of windows is heat transfer by convection between the interior and exterior surfaces and their respective environments. In particular, a better understanding of wind and thermal induced convection heat transfer at the exterior surface is needed to resolve the present discrepancies in window thermal testing. The report presents the result of an extensive search of the English-language literature for publications relevant to the phenomena of convection from windows.

*600,070*

**PB86-189891** PC **A08**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Building Energy Analysis with BLAST and CEL-1,**
S. J. Treado, D. B. Holland, W. E. Remmert, and W. Pierpoint. Feb 86, 174p NBSIR-85/3256
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Daylighting, Buildings, Illuminating, Solar radiation, Computer programs, *Energy analysis, Energy consumption.

The report describes the capabilities of the BLAST and CEL-1 computer programs and the procedures for using a hybrid version which incorporates both programs into a single design and analysis tool. Details on assembling the required information for development of the input files and the actual execution of the hybrid program are covered. The program allows detailed simulation of actual lighting systems using CEL-1 including daylighting effects while providing BLAST with lighting energy modifiers on an hourly basis. The procedure is demonstrated using a sample building.

*600,071*

**PB86-189909** PC **A10**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**HVACSIM+ Building Systems and Equipment Simulation Program: Building Loads Calculation,**
C. Park, D. R. Clark, and G. E. Kelly. Feb 86, 203p NBSIR-86/3331
See also PB86-130614. Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems, and Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Environmental engineering, *Buildings, Computerized simulation, Building systems, HVACSIM(+) computer program.

A non-proprietary building system simulation program called HVACSIM+, which stands for HVAC SIMulation PLUS other systems, has been developed at the National Bureau of Standards (NBS) in an effort to understand the dynamic interactions between a building shell, an HVAC system, and building controls. HVACSIM+ consists of a main simulation program, a library of HVAC system component models, a building shell model, and interactive front end input data generation programs. The report presents the overall architecture of the HVACSIM+ program, algorithms used in the main simulation program, a brief discussion of the numerical methods used in solving a system of non-linear simultaneous equations, integrating stiff ordinary differential equations and interpolating data and descriptions of the building shell and zone models.

*600,072*

**PB86-196300** PC **A07**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Linear Opponent-Colors Model Optimized for Brightness Prediction.**
Final rept.,
G. L. Howett. Feb 86, 127p NBSIR-85/3202

Keywords: *Illuminating, *Brightness, Color, Mathematical models, Luminance, Color vision, Optimization.

Formal multivariate optimization techniques were applied in an attempt to determine how well a linear, opponent-colors model of color vision could account for specific brightness-matching data. The data fitted were from a single experiment by Sanders and Wyszecki that matched an adjustable white light in brightness to each of a set of lights of 96 different colors and constant luminance. A generalized, linear, opponent-colors model was formulated, which included the models of Guth (and co-workers), Ingling (and co-workers), and Thornton as special cases. The model contained 10 parameters, including nine determining the spectral responses of the three opponent-level channels and one determining the rule for combining the outputs of the three channels to obtain an estimate of equivalent luminance (the luminance of an equally bright white light). Despite difficulties with the optimization procedure, a model was found that correlates better than 0.98 with the fitted data. The predictions of the model for various other color-vision functions were explored and compared with corresponding predictions of the Guth and Lodge model and the Thornton model.

*600,073*

**PB86-196466** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

**Applications of Aerial Thermography for Residential Energy Analysis.**
Final rept.,
S. J. Treado, and D. M. Burch. 1983, 1p
Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems.
Pub. in ASHRAE (American Society of Heating, Refrigeration and Air-Conditioning Engineers) Jnl. EN 25, n5 p52 1983.

Keywords: *Residential buildings, Aerial photography, Heat loss, Reprints, *Energy analysis, *Infrared thermography.

The effectiveness of aerial infrared thermography as a residential energy analysis procedure is investigated. Factors affecting the accuracy and utility of the technique are identified and analyzed, including the effects of location microclimate and different thermostat setpoints. Guidelines are presented concerning the recommended use of aerial thermography as a procedure for assessing the thermal performance of residences.

*600,074*
**PB86-196755** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Sky Luminance and Direct Beam Illuminance,**
S. J. Treado, W. E. Remmert, and J. W. Bean. Mar 86, 51p NBSIR-85/3251

Keywords: *Sky, *Luminance, *Daylighting, Irradiance, Illuminance, Measurement, Beams(Radiation).

Measurement of sky illuminance, sky luminance, direct beam illuminance and direct beam irradiance are analyzed and discussed. The database consisted of an annual set of integrated hourly measurements made at the National Bureau of Standards, Gaithersburg, Maryland. The relationship between diffuse sky illuminance and luminance of selected portions of the sky dome is examined. Measured sky luminances are compared to luminance calculated using equations for three standard sky types-clear, partly cloudy and overcast. The results indicate that the luminance distribution of actual skies varies considerably from the standard skies.

*600,075*
**PB86-203593** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Low-Cost Measurement of the Air Leakage in Homes.**
Final rept.,
G. T. Linteris, and A. K. Persily. 1984, 2p
Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.
Pub. in Proceedings of Summer Study in Energy Efficient Buildings, Santa Cruz, CA., August 22, 1982, p547-548 1984.

Keywords: *Residential buildings, Air, Leakage, Pressurizing, Tests, Measurement, *Air infiltration.

Simultaneous air infiltration measurements were performed in a group of fourteen nominally identical wood frame houses located in New Jersey, for three test periods. The results of the measurements indicate that there was more than a two to one variation in infiltration between the houses. The fourteen houses were pressure tested using the Blower Door apparatus, and these results are also presented. Comparisons are made between the two measurement techniques. Several state-of-the-art air infiltration predictive models are used to predict the air infiltration rates in the houses and these are compared with the measured infiltration rates.

*600,076*
**PB86-210093** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Measurement-Based Calculation of Infiltration in Passive Solar Performance Evaluation.**
Final rept.,
B. Hamilton, B. Sachs, J. Duffy, and A. Persily. 1983, 6p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of National Passive Solar Conference (8th), Sante Fe, NM., September 7-9, 1983, Progress in Passive Solar Energy Systems, v8 p295-300.

Keywords: *Residential buildings, Fluid infiltration, *Solar energy.

Low-cost, measurement-based techniques for calculation of infiltration as a variable in passive solar performance evaluation are suggested as an improvement over the use of an assumed constant air-change rate. Results of infiltration measurements and calculations are reported for 70 passive solar homes. Comparisons are made between two infiltration estimation techniques for 41 of these monitored buildings.

*600,077*
**PB86-229598** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Comparison of Measured and Predicted Sensible Heating and Cooling Loads for Six Test Buildings,**
D. M. Burch, G. N. Walton, B. A. Licitra, and K. Cavanaugh. Jun 86, 29p NBSIR-86/3399
Sponsored by Electric Power Research Inst., Palo Alto, CA.

Keywords: *Heating loads, *Cooling loads, Residential buildings, Evaluation, Energy conservation.

Hourly sensible heating and cooling loads for six test buildings were predicted using two computer programs, called TARP and EMPS. The predicted loads were compared to corresponding measured loads for winter heating, spring heating, and summer cooling periods. Both computer programs predicted the general trends of the measured data.

*600,078*
**PB87-106746** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Dynamic Models for HVAC System Components.**
Final rept.,
D. R. Clark, C. R. Hill, and C. W. Hurley. 1985, 10p
Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems, and Civil Engineering Lab. (Navy), Port Hueneme, CA.
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 1B, p737-746 1985.

Keywords: Computerized simulation, Mathematical models, Heat exchangers, Ducts, Pipes(Tubes), Reprints, *Space HVAC systems.

A method for representing transport delays is presented, and dynamic models for a pipe or duct and for a hot water coil are derived. Briefer descriptions of models for several other components of an air handler are given. Comparisons between experimental data and simulation results are provided to support the validity of the models. Detailed simulations of a complete heating coil control loop serve as the basis for experimental verification of the component models and their interactions.

*600,079*
**PB87-108098** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Thermal and Services Systems Div.
**Assessment of Retrofitting Automatic Vent Dampers on Oil-Fired Residential Heating Systems in the New England Area.**
Final rept.,
L. Katzman, G. E. Kelly, and M. E. Kuklewicz. 1978, 7p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Conference on Documentation and Analysis of Improvements in Efficiency and Performance of HVAC Equipment and Systems, West Lafayette, IN., October 23-25, 1978, p180-186.

Keywords: *Residential buildings, *Heating, Vents, Boilers, Furnances, Fuels, Savings, *Draft control systems, New England.

A field study involving the installation of twenty-one automatic vent dampers on oil-fired, residential furnaces and boilers in the New England area is described. Good agreement is shown to exist between the measured percent fuel savings, obtained by comparing test periods before and after modification, and the percent fuel savings predicted using an NBS recommended procedure for determining the part load and seasonal efficiency of such equipment. The NBS procedure is then used to generalize the results to an average U.S. climate and a fixed heating system oversizing of 70 percent. Information is also presented on various problems encountered during the study with the installation of automatic vent dampers on oil-fired residential furnaces and boilers.

*600,080*
**PB87-115440** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Solar Energy Absorption by Vertical Cylindrical-Tube Absorbers in Sunspace Enclosures.**
Final rept.,
M. E. McCabe, and M. van Migom. 1983, 8p
Sponsored by Department of Energy, Washington, DC. Passive and Hybrid Solar Energy Div.
Pub. in Proceedings on Winter Annual Meeting of the American Society of Mechanical Engineers, Boston, MA., November 13-18, 1983, 8p.

Keywords: *Solar heating, *Buildings, Enclosures, Energy absorption, *Passive solar heating systems, *Solar absorbers.

Solar energy absorption in a building sunspace having a south-facing glazing and a row of parallel, uniformly-spaced, vertical, cylindrical solar absorbers is considered. The opaque cylindrical absorbers might be a part of a passive solar heating system which contains features of both a direct-gain and a collector-storage wall system. Considerable control over the gain of direct solar energy and thermal energy storage within a building space can be achieved by varying the diameter and spacing of the cylindrical tubes. A two-dimensional model is formulated for a horizontal, planar enclosure in which the cylinderical absorber tube is subdivided uniformly into a number of surface elements and the glazing and sunspace surfaces are each represented as single surface elements. The results are presented as dimensionless ratios of absorbed-to-incident solar flux. Plots of the spatial distribution of absorbed solar flux are presented for hourly time increments for a winter day.

*600,081*
**PB87-117974** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Probabilistic Models of Snow Loads on Structures.**
Final rept.,
B. Ellingwood, and M. O'Rourke. 1985, 9p
Pub. in Structural Safety 2, n4 p291-299 1985.

Keywords: *Buildings, *Loads(Forces), Climatology, Snow, Building codes, Design standards, Statistical analysis, Roofs, Probability distribution functions, Reprints.

Snow loads provide the governing load requirements for the structural design of roofs in many northern climates or mountainous regions. Current design practice in most countries is to calculate the roof snow load as the product of a ground load and a dimensionless ground-to-roof conversion factor. Both parameters are random variables, and appropriate fractiles of their distributions must be determined for use in design codes. Statistical data are presented on the ground snow obtained from analysis climatological data, and on ground-to-roof conversion factors measured by surveys of snow accumulation on roofs. These data are proving valuable in structural code development.

*600,082*
**PB87-118071** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Part-Load Performance Characteristics of Residential Absorption Chillers and Heat Pumps.**
Final rept.,
D. A. Didion, and R. Radermacher. 1984, 6p
Sponsored by Department of Energy, Washington, DC., and Oak Ridge National Lab., TN.
Pub. in Int. Jnl. Refrig. 7, n6 p393-398 1984.

Keywords: *Heat pumps, *Air conditioners, Absorption, Degradation, Loads(Forces), Testing, Reprints.

A series of laboratory performance tests were conducted on an absorption cycle water chiller and heat pump. The part-load performance was compared to the full-load capacity and coefficient of performance. The causes of performance degradation with shorter operating times are speculated upon with partial substantiation resulting from tests on the chiller after it had been modified to prevent off cycle fluid migration.

*600,083*
**PB87-120234** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

**Measurement and Quantification of Thermal Bridges in Four Office Buildings.**
Final rept.,
R. A. Grot, K. W. Childs, J. B. Fang, and G. E. Courville. 1985, 16p
Pub. in American Society of Heating, Refrigerating and Air-Conditioning Engineers Transactions 91, Pt 1B p558-573 1985.

Keywords: *Office buildings, *Heat loss, Heat transfer, Measurement, Conduction, Reprints, Energy conservation, Heat flow.

Thermal bridges are highly conductive heat flow paths within the building envelopes. The effects of thermal bridges on the overall heat loss through a building envelope are described. Thermally deficient areas caused by thermal bridges were found and their sizes ascertained in four office buildings by means of infrared thermography. Quantification of the heat loss caused by thermal bridging was achieved using field data obtained with heat flux transducers, along with a detailed analysis of the exterior thermographs and architectural drawings of the buildings involved. Field data were compared with the predictions obtained using a two-dimensional heat transfer model of the transient heat conduction within the exterior wall-floor system.

*600,084*
**PB87-120242** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**In situ Measurement of the Thermal Resistance of Building Envelopes of Office Buildings.**
Final rept.,
J. B. Fang, and R. A. Grot. 1985, 15p
Pub. in American Society of Heating, Refrigerating and Air-Conditioning Engineers Transactions 91, Pt 1B p543-557 1985.

Keywords: *Office buildings, *Thermal resistance, Measurement, Heat loss, Reprints, Energy conversation.

The thermal resistances of various sections of building envelopes in seven office buildings have been determined using heat flow meters and a portable calorimeter during the winter heating season. These buildings are situated in various climatic zones of the United States. They have exterior masonry walls of different types of design and constructions. The effects of the length of measurement period, and the time lag between the air temperature difference across the envelope and the heat flow on the results of in-situ thermal resistance measurements are discussed. The thermal resistance values derived from data obtained with the calorimeter are generally lower than those by heat flow meters due to additional heat losses associated with the framing members. In general, the measurement accuracy can be improved through correction for time lag. Reliable thermal resistance data are obtainable if the duration of heat flow and air temperature measurements is at least 24 hours. These resistance values departed from the predicted values by an average of 14%, the worst case being 45%.

*600,085*
**PB87-122461** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Window Glass Facades as Structural Systems: An Improved Reliability-Based Design Procedure.**
Final rept.,
E. Simiu, and A. Filotti. 1985, 10p
Pub. in Proceedings of the International Conference on Structural Safety and Reliability ICOSSAR '85 (4th), Kobe, Japan, May 27-29, 1985, 10p.

Keywords: *Window glass, Architecture, Buildings, *Wind loads.

The purpose of the paper is to present a risk-consistent procedure for the design of glass cladding facades subjected to wind loads. The procedure is applicable to buildings with specified orientation, and accounts in a probabilistically rigorous manner for the dependence upon wind direction of both the extreme wind speeds and the pressure coefficients. In addition, the procedure is consistent with the fact that both the wind loads acting on various panels and the load capacities of the panels may be mutually correlated. It is shown that, depending upon building orientation, the procedure presented here can lead to significant reductions in the cost of glass cladding facades while ensuring safety levels at least as high as those inherent in current practice.

## Building Equipment, Furnishings, & Maintenance

*600,086*
**PB87-128070** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Air Infiltration Site Measurement Techniques.**
Final rept.,
D. T. Harrje, R. A. Grot, and D. T. Grimsrud. 1982, 19p
Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.
Pub. in Proceedings of the Air Infiltration Centre Conference on Building Design for Minimum Air Infiltration (2nd), Stockholm, Sweden, September 21-23, 1981, p115-133 1982.

Keywords: *Buildings, Measurement, Measuring instruments, *Air infiltration, *Tracer techniques, Computer applications.

A summary of the existing types of air infiltration measurement techniques and instrumentation using tracer gases is presented. Automated air infiltration instrumentation used by researchers in the United States, Canada, the United Kingdom, Denmark, Sweden, and Switzerland is described. The equipment can operate in the dilution (decay) mode, constant flow mode and the constant concentration mode. Most of these instruments are microcomputer or microprocessor based and capable of performing real time determination of the air infiltration rate in multizone buildings and monitor the state of additional parameters such as temperature, wind speed and energy consumption. Two simple techniques, the air bag or container method and the average infiltration monitor, developed by researchers in the United States are summarized.

*600,087*
**PB87-134326** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Specifications for Thermal and Environmental Evaluations of Advanced-Technology Office Buildings,**
A. K. Persily. Nov 86, 96p NBSIR-86/3462
Sponsored by Public Buildings Service, Washington, DC.

Keywords: *Office buildings, Evaluation, Specifications, *Energy management, *Environmental engineering, *Federal buildings, US GSA.

Specifications for conducting a thermal and environmental evaluation program for advanced technology office buildings are presented. The program is to be used by the General Services Administration (GSA) in designing and assessing the performance of these new federal office buildings. The document consists of three basic sections: (1) programing directives - a description of requirements regarding the diagnostic center and associated items, and quantitative architectural performance standards, to be used in the building design process; (2) construction specifications - detailed specifications regarding the procurement and installation of sensors and equipment for use in the evaluations, written in the Masterspec format developed by the Construction Specifications Institute; (3) work statements - detailed descriptions of each of the thermal and environmental evaluations for use in procuring the services of individuals or organizations to perform the tests. The three sections are intended for use by GSA in the design and procurement processes, and are therefore presented in formats appropriate to GSA's needs.

*600,088*
**PB86-185311** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Need and Availability of Test Methods for Measuring the Smoke Leakage Characteristics of Door Assemblies.**
Final rept.,
L. Y. Cooper. 1986, 20p
See also PB84-216480. Sponsored by Department of Health and Human Services, Washington, DC., Bureau of Mines, Washington, DC., and National Park Service, Washington, DC.
Pub. in ASTM (American Society for Testing and Materials) Special Technical Publication 882, p310-329 1985.

Keywords: *Doors, *Smoke, *Leakage, Buildings, Reprints, Compartment fires.

The paper identifies and places into perspective relevant information that would assist in focusing future research and development on test methods to measure the smoke leakage characteristics of door assemblies. The concept of smoke compartmentation is introduced and developed. The importance of cross-door pressure differential in establishing the performance of door assemblies in fire-generated environments is discussed. Door assembly performance then is related to life safety, in general, and to the design of compartments of safe refuge, in particular. The entire discussion suggests a listing of required door assembly test methods and, finally, leads to a review of the availability and development status of existing and potential future test method candidates.

*600,089*
**PB86-185675** PC **A05**/MF **A01**
Dayton Univ., OH. Research Inst.
**Mathematical Modeling of Furniture Fires.**
Interim rept.,
M. A. Dietenberger. Feb 86, 83p NBS/GCR-86/506
Grant NB83NADA-4056
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Furniture, *Flammability, Burning rate, Flame propagation, Flammability testing, Fire damage, Mathematical models, Fire models.

The objective of the work was to develop a working computer model of a furniture fire which utilizes the bench scale measurements on furniture samples of burning rate history, flame spread rate, time to ignition, and the fraction of fuel converted to soot. The primary prediction of the model was to be the burning rate of a furniture fire as a function of time.

*600,090*
**PB86-196326** PC **A08**/MF **A01**
Stanford Univ., CA. Dept. of Aeronautics and Astronautics.
**Behavior of Furniture Frames during Fire. Final Report,**
G. S. Springer. Apr 86, 162p NBS/GCR-86/512
Contract NB83-NAD-4019
See also PB86-102225. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Furniture, *Fires, Frames, Fire studies.

The objective of the investigation was to evaluate the behavior of furniture frames during exposure to elevated temperatures such as may arise in fires. An analytic method was developed for calculating stresses and strains in wooden beams and bends at elevated temperatures. Models were established for calculating the degradation in strength of wood due to elevated temperature exposure and for predicting the times to failure of loaded wooden structures.

*600,091*
**PB86-196409** PC **A07**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Initial Test Results and Test Plan for Differential Temperature Controllers Used in Solar Energy Systems.**
Final rept.,
J. Greenberg. Apr 86, 145p NBSIR-86/3346
Contract DE-AI01-76PR06010
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: *Temperature control, Control equipment, Cooling systems, Heating, Controllers, *Solar heating systems, *Solar cooling systems.

The initial test results and procedures used to conduct tests on differential temperature controllers used in solar energy systems are discussed. These tests were performed on generally non-adjustable, non-display units and include the following functional tests conducted at ambient conditions: delta T 'on' and 'off'; recirculating freeze protection with and without auxiliary sensor; controller response to sensor sensitivity; storage high temperature limit; and pump 'off' below 80 C.

Controller sensitivity to line voltage variation tests were also conducted at ambient conditions and include: delta T 'on' and 'off' and recirculating freeze protection. The controller test fixture is also described along with the recommended use of decade resistance boxes to simulate thermistor inputs. An overall test plan is also included as an appendix to the report.

*600,092*
**PB86-210721** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Evaiuation of Furniture Fire Hazard Using a Hazard-Assessment Computer Model.**
Final rept.,
R. W. Bukowski. 1985, 8p
Pub. in Fire and Materials 9, n4 p159-166 1985.

Keywords: *Furniture, *Fire hazards, Fire resistant coatings, Upholstery, Residential buildings, Toxicity, Burning rate, Smoke, Reprints.

The Center for Fire Research Fire (Toxic) Hazard-Assessment computer model was used to evaluate the potential for hazard reduction by the modification of the combustion properties of upholstered furniture items in a residential occupancy. The potential benefits of these modifications are compared with the effects of variations in room size and construction to determine if they would be realized across a range of housing sizes and types. The results demonstrate the greatest benefit by the reduction of the mass loss (burning) rate of the item regardless of room size and even if the means used to reduce the burning rate results in an increase in smoke production and material toxicity.

*600,093*
**PB87-101002** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Relative Propensity of Seiected Commercial Cigarettes to ignite Soft Furnishings Mockups,**
J. F. Krasny, and R. G. Gann. Jun 86, 57p NBSIR-86/3421
Sponsored by Consumer Product Safety Commission, Washington, DC.

Keywords: *Furniture, *Fabrics, *Ignition, Upholstery, Tests, *Cigarettes.

The report covers the first project performed under the Cigarette Safety Act of 1984, the determination of whether and to what extent commercial cigarettes have differing propensities to ignite upholstered furniture substrates. For this purpose, a test was developed under which 12 types of commercial cigarettes were placed on 18 substrates varying in fabric, padding, and configuration. It was found that there are statistically significant differences in ignition propensity among the cigarettes on three substrates. No significant differences were found on the other 15 substrates. However, no one of the packings consistently showed low ignition propensity on all three substrates. The mass loss rate of both the cigarette and substrate during the tests was recorded and did not appear to be a reliable predictor of ignition propensity.

*600,094*
**PB87-128138** Not available NTiS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**New Approach to Fire Toxicity Data for Hazard Evaiuation.**
Final rept.,
V. Babrauskas, B. C. Levin, and R. G. Gann. 1986, 6p
Pub. in American Society for Testing and Materials Standardization News 14, n9 p28-33 Sep 86.

Keywords: *Fires, *Toxicity, *Combustion products, Tests, Hazards, Models, Reprints, Cone calorimeters.

An N-gas model involving a reduced dependence on animal testing is proposed both for obtaining fire toxicity data for hazard modeling and for premarketing screening of commercial products and materials. Current toxicity measures rely almost exclusively on animal testing. The proposed new approach is based on obtaining the time-dependent generation rates of a limited number of important toxic species using a suitable combustion apparatus, such as the Cone Calorimeter. The new approach will not entirely eliminate the need for animal testing, since a check-test will still be necessary, but it promises to substantially reduce the need for animals.

*600,095*
**PB87-128153** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Quarter-Scale Room Fire Tests of Interior Finishes.**
Final rept.,
B. T. Lee. 1985, 7p
Pub. in Fire and Materials 9, n4 p185-191 1985.

Keywords: *Finishes, *Fires hazards, *Buildings, Model tests, Flashover, Ignition, Reprints.

A technique for modeling fire buildup in rooms with combustible interior finish is discussed. Use of the technique resulted in good agreement between fires conducted in one-quarter scale model rooms with a doorway opening and those performed in full-scale rooms. The effects of burner location and heating rate on flashover in a well-insulated room were also studied to help select a suitable ignition source size and placement for testing of interior finish materials.

*600,096*
**PB87-128161** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Standard Room Fire Test Development at the National Bureau of Standards.**
Final rept.,
B. T. Lee. 1985, 16p
Pub. in American Society for Testing and Materials Special Technical Publication 882, p29-44 1985.

Keywords: *Finishes, *Fire tests, *Buildings, Plywood, Polystyrene, Gypsum, Evaluation, Flashover, Thermal radiation, Calorific value, Heat of combustion, Reprints.

Research results with the proposed ASTM standard room fire test for interior finish materials are presented. The materials selected for the study were two untreated plywoods, a fire-retarded plywood, polystyrene, polyisocyanurate, and gypsum board. Three 900 s duration test scenarios were considered. The study demonstrated that all three scenarios could adequately differentiate material fire behavior, in terms of the maximum degree of fire buildup attained and the time to reach the maximum, for the materials selected. Thermal radiation incident on the floor and doorway air temperature were found to be the most consistent parameters for determining room fire buildup including room flashover. Surface flame spread and rate of heat release are presented for the room fires. Unit area rate of heat release from these fires were found to correlate marginally with calorimeter data for the same materials.

*600,097*
**PB87-134292** PC **A08**/MF **A01**
Case Western Reserve Univ., Cleveland, OH. Dept. of Mechanical and Aerospace Engineering.
**Discharge Distribution Performance for an Axisymmetric Model of a Fire Sprinkler Head,**
B. Wendt, and J. M. Prahl. Oct 86, 170p NBS/GCR-86/517
Contract NB82-NADA-3038
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Fire safety, *Sprinklers, Droplets, Computer programs, Graphs(Charts), Performance, Models, Water sprays.

A nondimensional description of spray discharge distribution performance of fire sprinkler heads is developed. The description emphasizes the sprinkler's ability to evenly distribute the spray over the maximum possible floor area. Illustration of the description is provided by data obtained from an apparatus developed to study the axisymmetric jet impingement on a flat disk. The apparatus employs the disintegration of an axisymmetric film to produce the droplet spray. Sheet breakup radius varies as the inverse one third power of the Weber number based on jet diameter, in agreement with data obtained by Huang. Variable discharge distribution performance is achieved by controlled axial vibrations of the disk. Identical nondimensional distributions are obtained at a frequency ratio defined as the ratio of the driving frequency to the frequency of maximum growth of sinuous waves, as outlined by Squire. A spray modelling procedure is developed to give analytical discharge distributions. An investigation of the resulting patterns indicates a volume mean droplet diameter in agreement with a predicted value obtained from a correlation given by Dundas and Huang.

## Building Standards & Codes

*600,098*
**PB86-195583** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Expressing Standards for Computer-Aided Building Design.**
Final rept.,
F. I. Stahl, R. N. Wright, S. J. Fenves, and J. R. Harris. 1983, 6p
Pub. in Computer Aided Design 15, n6 p329-334 Nov 83.

Keywords: *Buildings, *Building codes, Design, Standards, Reprints, Computer-aided-design.

The article discusses a set of techniques for expressing and organizing the contents of building design standards, and suggests that application of these techniques, in conjunction with a restructuring of data flow strategies within computer-aided building design (CABD) software systems, are needed to reduce the effort and cost required to maintain CABD systems applicable and current. The article stresses application of these techniques to analyzing the clarity, consistency, and completeness of existing building design standards, and to developing new standards.

*600,099*
**PB86-199924** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Probability-Based Load Criteria for Structural Design.**
Final rept.,
B. Ellingwood. 1985, 10p
Sponsored by American Society of Civil Engineers, New York.
Pub. in Proceedings of Concepts and Methods in Structural Safety Studies, Denver, CO., April 27-May 3, 1985, p120-129.

Keywords: *Building codes, *Structural design, Loads(Forces), Design standards, Structural engineering.

Load criteria for use in limit states design of structures are developed using probabilistic methods. Statistical data on load and strengths are integrated by the reliability analysis to yield criteria that are consistent with a prescribed measure of reliability. The load criteria, while having a conventional appearance, lead to more uniform reliability and performance than is possible with existing specifications. The load criteria have been included in American National Standard A58.1-1982, Minimum Design Loads for Buildings and Other Structures, and provide a focus for material specification writers as limit states design methods are developed for different construction materials.

*600,100*
**PB86-199940** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Standards Interface for Computer-Aided Design: An Overview of Some Technical Probiems Associated with Automated Design Checking.**
Final rept.,
F. I. Stahl. 1984, 8p
Pub. in Proceedings of Conference on Computing in Civil Engineering (3rd), San Diego, CA., Aprii 2-6, 1984, p560-567.

Keywords: *Building codes, *Design standards, Structural design, Structural engineering, *Computer aided design.

Building quality can be improved and building costs reduced through more effective computer utilization in design and construction. To accomplish these objectives improved interfaces are needed between building project databases and computer-based procedures for analysis and design, and between computer-based engineering procedures and applicable design standards. The report examines the hypotheses that: (1) the ability to easily maintain design standards data is fundamental to CAD system effectiveness; (2) the config-

uration of presently available computer-aided structural design (CASD) system software inhibits efficient design standards data modification, requiring costly maintenance to avoid software obsolescence and limiting the overall usefulness of these systems; and (3) methods to enhance the efficiency of criterion checking and standards data maintenance are required to increase the utilization of CAD technology.

*600,101*
**PB86-230968** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Regulatory Response to Technical Innovation in Residential Construction.**
Final rept.,
F. T. Ventre. 1984, 9p
Pub. in Proceedings of HUD/NIBS Conference on Next Generation of Housing Technology, Orlando, FL., April 26-27, 1982, p83-91 1984.

Keywords: *Residential buildings, *Construction, Regulations, Standards, Construction industry, Control, Regulations.

Describes varieties of regulation, their uses and abuses and their effects on the wider use of innovative technology in residential building construction. Offers frameworks for resolving regulatory questions and describes NBS contributions to regulatory reform.

*600,102*
**PB87-105219** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Improving Building Regulations for Rehabilitation.**
Final rept.,
J. C. Gross. 1985, 14p
Pub. in Proceedings of ACI Symposium on Rehabilitation, Renovation and Preservation of Concrete and Masonry Structures, Quebec City (Canada), 20-25 September 1981, p121-134 1985.

Keywords: *Building codes, Renovating, Regulations, Reconditioning, Maintenance.

The purpose of the paper is to provide an overview of building regulations applied to rehabilitation. Discussed are (1) constraints due to regulation, (2) recent technical activity to improve rehabilitation regulation, and (3) needed research to permit more effective use of our existing building stock.

*600,103*
**PB87-108627** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Overview of Building Regulations That Relate to Rehabilitation.**
Final rept.,
J. H. Pielert. 1982, 9p
Pub. in Evaluation, Maintenance, and Upgrading of Wood Structure, Ch1.6 p39-47 1982.

Keywords: *Buildings, *Regulations, *Rehabilitation.

No abstract available.

## Construction Materials, Components, & Equipment

*600,104*
**PB86-192408** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Slide Rule Estimates of Fire Growth.**
Final rept.,
J. R. Lawson, and J. G. Quintiere. 1985, 26p
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.
Pub. in Fire Technology 21, n4 p267-292 Nov 85.

Keywords: *Fires, *Flame propagation, Estimates, Smoke, Reprints, Fire models, Compartment fires.

A series of prediction methods has been assembled to provide an analytical basis for estimating fire growth in compartments. Solutions for each prediction method can be made using programmable scientific calculators. Prediction methods are presented for: fire size and growth rates, mass loss rates, radiant heat flux, flame height, radial flame impingement, heat flux to a ceiling, smoke filling of a room, carbon monoxide hazard with smoldering fires, temperature rise in a compartment, ventilation flow rate, flashover occurrence, corridor smoke transfer and filling, smoke concentration, visibility, flame spread rates, and fire burn time.

*600,105*
**PB86-192499** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Finite-Element Analysis of Temperature-Induced Stresses in Single-Ply Roofing Membranes.**
Final rept.,
W. J. Rossiter, and M. E. Batts. 1985, 14p
Pub. in Durability of Building Materials 2, n3 p195-208 Jan 85.

Keywords: *Roofing, *Thermal stresses, Finite element analysis, Stress analysis, Reprints.

A linear finite-element method of analysis was used to calculate stresses induced in a single-ply roofing membrane by thermal gradients through the roof system. The roofing system in the analysis consisted of a totally adhered or loose-laid EPDM membrane, two layers of fibrous glass insulation board, and a metal deck.

*600,106*
**PB86-196334** PC **A04**/MF **A01**
Pennsylvania State Univ., University Park. Dept. of Mechanical Engineering.
**Model for Vertical Wall Fire in a Stratified Atmosphere.**
Annual rept. 15 Aug 84-14 Aug 85,
A. K. Kulkarni, and J. Hwang. Mar 86, 63p NBS/GCR-86/510
Contract NANB-4D0037
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Fires, Mathematical models, Laminar flow, Walls, Flammability testing, *Fire models, *Fire studies, Compartment fires.

A comprehensive mathematical model is presented for understanding the characteristics of a burning vertical wall immersed in a quiescent ambient atmosphere having a nonuniform vertical distribution of temperature and oxidizer mass fraction. Such a stratified atmosphere occurs, for example, in the interior of a room or aircraft cabin on fire. A set of partial differential equations and suitable boundary conditions describing a laminar flow of exothermically reacting species is solved using the Keller Box finite difference scheme. Results of burning rate and flow parameters (such as the maximum vertical velocity, flame position, etc.) are presented for many different cases of stratified atmosphere.

*600,107*
**PB86-196573** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Assessment of Accuracy of In-situ Methods for Measuring Building Envelope Thermal Resistance,**
J. B. Fang, R. A. Grot, and H. S. Park. Mar 86, 28p NBSIR-86/3328
Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.

Keywords: *Thermal resistance, *Buildings, Insulation, Thermal insulation, Heat flux, Calorimeters, Thermal measurements, Field tests.

A series of field and laboratory tests were conducted to evaluate the accuracy of in-situ thermal resistance measurement techniques. The results of thermal performance evaluation of the exterior walls of six thermal mass test houses situated in Gaithersburg, Maryland are presented. The wall construction of these one-room houses includes insulated light-weight wood frame, uninsulated light-weight wood frame, insulated masonry with outside mass, uninsulated masonry, log, and insulated masonry with inside mass. In-situ measurements of heat transfer through building envelopes were made with heat flux transducers and portable calorimeters.

*600,108*
**PB86-196631** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Effect of Age Upon Diffusion in Hydrated Alite Cement.**
Final rept.,
L. J. Parrott, R. G. Patel, D. C. Killoh, and H. Jennings. 1984, 5p
Pub. in Jnl. of the American Ceramic Society 67, n4 p233-237 1984.

Keywords: *Cements, Diffusion, Porosity, Microstructure, Calcium sillicates, Permeability, Reprints, *Alite.

The diffusion properties of hydrated alite cement have been compared with measurements of the degree of hydration and of pore structure for a range of ages. During hydration the large pores in the hydrated alite were progressively filled with a porous calcium silicate hydrate gel. At early stages of hydration the larger pores were directly interconnected and diffusion rates were consequently rapid. At later stages of hydration the hydrate shells around adjacent alite grains began to intergrow continuity of the larger pores is reduced. Diffusion rates then deminish rapidly with only small amounts of additional hydration. Quantitative microscopy, thermogravimetric analysis, calorimetry, quantitative X-ray diffraction and butane adsorption were used to study the microstructural development in the hydrating alite. Geometric and spacial characteristics of the pores in the hydrated alite were investigated by microscopic examination of resin replicas.

*600,109*
**PB86-200367** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Prediction of Upholstered Chair Heat Release Rates from Bench-Scale Measurements.**
Final rept.,
V. Babrauskas, and J. F. Krasny. 1985, 17p
Pub. in Proceedings of Fire Safety: Science and Engineering, ASTM STP 882, p268-284 1985.

Keywords: *Chairs, *Flammability testing, *Fire safety, Fire tests, Seats, Upholstery, Furniture, Calorimeters, Fire studies.

In an earlier study a full-scale furniture calorimeter was used to determine the heat release rates for upholstered chairs containing various construction materials. Samples of these same material combinations have now been tested in a bench-scale apparatus, the cone calorimeter. A correlation was established between bench-scale and full-scale data. Thus, it appears that prediction of flashover potential of a single upholstered item may be possible by using bench-scale results.

*600,110*
**PB86-201027** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Buoyant Plume-Driven Adiabatic Ceiling Temperature Revisited.**
Final rept.,
L. Y. Cooper, and A. Woodhouse. 1985, 6p
See also PB85-200103. Sponsored by American Society of Mechanical Engineers, New York.
Pub. in Proceedings of National Heat Transfer Conference, Heat Transfer in Fire and Combustion Systems, Denver, CO., August 4-7, 1985, p167-172.

Keywords: *Fires, Convection, Heat transfer, *Plume-driven ceiling jet, Compartment fires, Fire models, Fire studies.

In previous works, convective heat transfer from buoyant plume-driven ceiling jets to unconfined ceilings has been estimated using a formula for the temperature distribution below an adiabatic ceiling.

*600,111*
**PB86-201795** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Service Life Prediction: The Barriers and Opportunities.**
Final rept.,
L. W. Masters. 1983, 11p
Sponsored by Conseil International du Batiment pour la Recherche l'Etude et la Documentation, Rotterdam (Netherlands).
Pub. in Proceedings of the Congress CIB 83 (Conseil International du Batiment pour la Recherche l'Etude et la Documentation) (9th), Stockholm, Sweden, August 15-19, 1983, p9-19.

Keywords: *Construction materials, Buildings, Degradation, Durability, Deterioration, Service life, Tests, *Foreign technology.

The need to advance the state of knowledge of service life prediction of building materials and, thereby, reduce a barrier to innovation and improved cost effectiveness has stimulated a number of internationally sponsored activities. The purpose of the paper is to identify some of the primary technical barriers and research opportunities that are presented to international groups working together to meet the need for improved service life predictions.

*600,112*
**PB86-202488** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD.
**Suggested Approaches for Revisions of Preliminary Performance Criteria for Tensile and Tensile Fatigue Strength Tests of Bituminous Membrane Roofing,**
H. W. Busching, W. J. Rossiter, and R. G. Mathey. Apr 86, 65p NBSIR-86/3347
Prepared in cooperation with Clemson Univ., SC. Dept. of Civil Engineering. Sponsored by Du Pont de Nemours (E.I.) and Co., Old Hickory, TN. Textile Fibers Dept.

Keywords: *Roofing, *Bitumens, Tensile strength, Tensile properties, Evaluation.

Alternative approaches are reviewed for revision of the original NBS preliminary performance criteria for tensile strength and tensile fatigue strength of bituminous membrane roofing. Reviews of five approaches - elasticity theory, brittle fracture, viscoelasticity theory, strain energy and finite element techniques - were completed. Advantages and limitations of these approaches were identified and use of the strain energy approach for both tensile strength and tensile fatigue strength preliminary performance criteria was recommended.

*600,113*
**PB86-203585** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Effect of Wall Mass and Insulation on Energy Consumption in Residential Buildings: An Experimental Study.**
Final rept.,
D. M. Burch. 1983, 11p
Sponsored by Conseil International du Batiment pour la Recherche l'Etude et la Documentation, Rotterdam (Netherlands).
Pub. in Proceedings of CIB Congress to Build and Take Care of What We have Built with Limited Resources (9th), Stockholm, Sweden, August 15-19, 1983, v3a, p245-255.

Keywords: *Residential buildings, Walls, Thermal insulation, *Energy consumption.

The paper investigates the effect of wall mass on the space heating and space cooling requirements of residential buildings. Six test buildings were extensively instrumented and subsequently exposed to outdoor climatic conditions near Washington, D.C. No reductions in space heating requirements attributed to wall mass were observed during the winter heating season when some space heating was provided each hour of the test. However, during the intermediate heating season and the summer cooling season, when the heating/cooling plant did not operate during a portion of the day, significant reductions in space heating/cooling requirements attributed to wall mass were observed.

*600,114*
**PB86-203601** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**NBS (National Bureau of Standards) Line-Heat-Source Guarded Hot-Plate for Thick Materials.**
Final rept.,
F. J. Powell, and B. G. Rennex. 1983, 16p
Sponsored by American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA.
Pub. in Proceedings of ASHRAE/DOE Conference on Thermal Performance of the Exterior Envelopes of Buildings 2, Las Vegas, NV., December 6-9, 1982, p657-672 1983.

Keywords: *Thermal measuring instruments, *Thermal insulation, Thermal resistance, *Guarded hot plate.

The use of higher R-value and thicker thermal insulation materials required NBS to produce a new apparatus for absolute measurements of thick materials that can be used as transfer standards. These standards are used for calibration of guarded hot-plate (ASTM C-177) or heat flow meter (ASTM C-518) equipment in user laboratories across the country. The paper gives a technical description of the as-built apparatus including dimensions and a summary of the rational used for the selection of the apparatus materials, the control instrumentation and the data logging equipment.

*600,115*
**PB86-203999** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Methodology for Assessing the Thermal Performance of Low-Sloped Roofing Systems,**
S. J. Treado, W. J. Rossiter, and R. G. Mathey. May 86, 51p NBSIR-85/3264
Sponsored by Department of Energy, Washington, DC.

Keywords: *Roofs, *Thermal analysis, Heat transmission, Moisture, Thermal resistance, Thermal efficiency, Energy conservation.

A methodology was developed to estimate the thermal performance of existing low-sloped roof systems. The methodology was based on a review of available information and experience. Roof system thermal resistance is used as the thermal performance characterization parameter. The procedure for determining total roof thermal resistance is described, including measurement and calculation methods, and adjustments for moisture intrusion, insulation gaps and fasteners.

*600,116*
**PB86-229515** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**NBS (National Bureau of Standards)/Harvard Mark VI Multi-Room Fire Simulation,**
J. A. Rockett, and M. Morita. May 86, 30p NBSIR-85/3281

Keywords: *Fire tests, Fires, *Compartment fires, Fire models, Fire studies.

The NBS/Harvard Mark VI multi-room fire simulation program structure is discussed and compared with Harvard V. In addition to the current, operating version of Mark VI, a development version is being used to test enrichments which can be readily moved into the operational version as they mature.

*600,117*
**PB86-245719** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Conference on Accreditation of Construction Materials Testing Laboratories, May 14-15, 1986. Executive Summary,**
J. H. Pielert. Jun 86, 28p NBSIR-86/3397
Sponsored by American Society for Testing and Materials, Philadelphia, PA.

Keywords: *Construction materials, *Materials specifications, *Meetings, Materials tests, Standards.

The Conference was structured to consider: The status of existing laboratory evaluation and accreditation programs; current trends in the accreditation process; and the need for and nature of a coordinated accreditation system. Included the presentation of invited papers and four workshop sessions.

*600,118*
**PB86-247889** PC **A03**/MF **A01**
Factory Mutual Research Corp., Norwood, MA.
**Spray Cooling in Room Fires.**
Technical rept.,
H. Z. You, H. C. Kung, and Z. Han. Jul 86, 46p NBS/GCR-86/515
Contract NB83-NADA-4054
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Fire tests, Ceilings(Architecture), Sprinklers, Cooling, Spraying, *Compartment fires, Room fires, Fire studies.

A series of 25 fire tests were conducted to investigate cooling in room fires by sprinkler spray. The tests were conducted in a test room, which had an opening centered in one of the 3.66 m walls. The fire source was a spray fire with constant heptane flow rate, located opposite the room opening. In each test only one sprinkler was installed at the ceiling.

*600,119*
**PB87-103321** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Modeling Window Optics for Building Energy Analysis,**
G. N. Walton. Jul 86, 50p NBSIR-86/3426
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: *Windows, *Optical tests, Daylighting, Heating, Energy conservation, Energy efficiency.

The report discusses modeling the optics of windows for the purposes of simulating building energy requirements or daylighting availability. The theory for calculating the optical performance of conventional windows is reviewed. The simplifications that might commonly be made in creating computational models are analyzed.

*600,120*
**PB87-104113** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Design of a Calibrated Hot-Box for Measuring the Heat, Air, and Moisture Transfer of Composite Building Walls.**
Final rept.,
P. R. Achenbach. 1981, 1p
Pub. in Proceedings of ASHRAE/DOE-ORNL Conference on Thermal Envelope of Buildings, Orlando, FL., December 3-5, 1979, p16 1981.

Keywords: *Buildings, Heat transfer, Walls, Thermal transfer.

A large calibrated hot-box is to be constructed at the National Bureau of Standards to support the development of standard procedures for measuring the heat, air and moisture transfer of room-size (3.0 by 4.5 m) exterior-wall specimens under a range of simulated climatic conditions. The apparatus will be used for research in both steady-state and dynamic thermal performance in support of standard test methods; for study of the processes of heat transfer, air leakage and moisture transfer in building walls as aids to the design and construction of buildings for energy conservation; and to provide traceability in measurement to NBS through calibration services, Standard Reference Materials or the National Voluntary Laboratory Accreditation Program.

*600,121*
**PB87-106738** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Moisture and Roof Performance.**
Final rept.,
D. M. Burch, R. G. Mathey, and W. J. Rossiter. 1984, 3p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 12, n11 p26-28 1984.

Keywords: *Roofs, *Moisture content, Roofing, Standards, Condensing, Reprints.

The article discusses moisture problems in ventilated attics of residential buildings and in low sloped roofing systems of industrial and commercial buildings. Existing standards relating to control of moisture are described. A synopsis of recent research on moisture problems in roofing systems is provided. The need for new standards is assessed.

*600,122*
**PB87-122784** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div.
**DATAPLOT as an Expert System for Interactive Data Analysis.**
Final rept.,
J. J. Filliben, and J. T. Fong. 1984, 19p
Pub. in Proceedings of 1984 ASME Pressure Vessels and Piping Conference and Exhibition, San Antonio, TX., June 17-21, 1984, v96 p37-55.

Keywords: *Computer graphics, Fortran, Microstructure, Quality control, Microcomputers, Construction materials, *Expert systems, *DATAPLOT system, Lan-

guage programming, Interactive systems, High level languages, Data analysis, Case studies.

A brief description of DATAPLOT(TM), a Fortran-based interactive, high-level language for data analysis and graphics, is presented. Capabilities of the most recent version (83/6) of DATAPLOT are described and illustrated with two examples. The use of DATAPLOT as an 'expert' system for 'advanced' data analysis, as implemented in a new version (84/6), is introduced through a case study involving the analysis of some microstructural data for use in the quality control of a rear axle housing casting of nodular cast iron. A discussion of the significance of the enhanced version of DATAPLOT is included.

*600,123*
**PB87-134839** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Window U-Values: Research Needs and Plans.**
Final rept.,
W. P. Goss, and M. E. McCabe. 1986, 7p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of ASHRAE/DOE/BTECC Conference on Thermal Performance of the Exterior Envelopes of Buildings III, Clearwater, FL., December 2-5, 1985, p716-722 1986.

Keywords: *Windows, Thermal conductance, Measurement, Thermal properties, Test methods, Transmittance, *U values.

Recently, there has been significant interest in developing a standard test procedure for determining the thermal transmittance (U-value) and thermal conductance (C-value) of window and window treatment products. Currently, several test methods are used to measure these quantities, and the proponents of these methods do not agree on a standard procedure for measurement. As a result, it is difficult to compare the U-values and overall thermal performance of different windows and window treatment products. The paper discusses the specific research needed to address the above problem, as well as a detailed two-phase program to perform that research.

*600,124*
**PB87-138376** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Strain Energy of Bituminous Built-Up Membranes: An Alternative to the Tensile Strength Criterion,**
W. J. Rossiter, and D. P. Bentz. Sep 86, 68p NBSIR-86-3418
Prepared in cooperation with Du Pont de Nemours (E.I.) and Co., Old Hickory, TN. Textile Fibers Dept.

Keywords: *Rooting, *Bitumens, *Tensile strength, Tension tests, Membranes, *Building materials.

The study was conducted to revise the performance criterion for tensile strength of bituminous built-up membranes. Bituminous membrane samples, fabricated from polyester fabric, polyester-glass composite fabric, and single plies of APP- and SBS-modified bitumen, were tested in tension to determine their load-elongation properties and to measure their strain energy. The results of the tensile tests of the new bituminous membranes indicated wide variability of load and elongation among the different types of materials.

## Structural Analyses

*600,125*
**PB86-164506** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Interdependence between Dynamic Surge Motions of Platform and Tethers for a Deep Water TLP (Tension Leg Platform).**
Final rept.,
E. Simiu, and A. Carasso. 1985, 6p
Sponsored by Minerals Management Service, Reston, VA.
Pub. in Proceedings of International Conference on Behaviour of Offshore Structures (BOSS '85) (4th), Delft, The Netherlands, July 1-5, 1985, p557-562.

Keywords: *Offshore structures, Dynamic response, Dynamic structural analysis, *Tetherlines.

The tethers of tension leg platforms (TLPs) undergoing surge motions are subjected to inertia and hydrodynamic loads. The purpose of the paper is to present an investigation into the effects of the tether curvature caused by these loads. The investigation is conducted by solving the coupled equations of surge motion of the tethers and of the platform.

*600,126*
**PB86-189065** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Dynamic Eccentricity of Structures Subjected to S-H Waves.**
Final rept.,
S. T. Wu, and E. V. Leyendecker. 1984, 10p
Pub. in Earthquake Engineering and Structural Dynamics 12, n5 p619-628 Sep/Oct 84.

Keywords: *Dynamic structural analysis, Structural analysis, Eccentricity, Seismic waves, Dynamic response, Reprints.

The paper presents the analytical result of a parametric study for a coupled lateral-torsional structural system subjected to seismic waves. Dynamic eccentricity is used as an index to represent the level of structural response. Case studies are provided to show the effects of a few parameters related to the characteristics of the structural systems. These parameters include the shape and size of the foundation mat. Accidental eccentricities due to seismic waves for the corresponding cases are also found and compared.

*600,127*
**PB86-192200** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Wind-Induced Motion of Tall Buildings.**
Final rept.,
A. Tallin, and B. Ellingwood. 1985, 8p
Pub. in Engineering Structures 7, n4 p245-252 1985.

Keywords: *Buildings, Skyscrapers, Wind pressure, Loads(Forces), Vibration, Reprints.

Modern buildings that are designed so that their lateral drifts under statically applied wind loads are less than some fraction of building height may vibrate excessively during winds and cause building occupants alarm. Methods are presented for evaluating the vibration characteristics of buildings using random vibration theory to relate the fluctuating wind forces to structural response.

*600,128*
**PB86-195013** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Analysis of Torsional Moments on Tall Buildings.**
Final rept.,
A. Tallin, and B. Ellingwood. 1985, 5p
Pub. in Jnl. of Wind Engineering and Aerodynamics 18, p191-195 1985.

Keywords: *Buildings, Skyscrapers, Torsional strength, Torque, Reprints, Wind tunnel tests.

Spectra of fluctuating wind forces on tall buildings can be determined experimentally from wind tunnel model tests either by measuring base torques using a force balance or by integrating the pressures measured on the sides of the model. The force balance technique is less costly, but may substantially overestimate the actual generalized forces. This study examines the relation between the spectra of base torques and generalized torques experienced by tall buildings.

*600,129*
**PB86-195203** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Wind-Induced Lateral-Torsional Motion of Buildings.**
Final rept.,
A. Tallin, and B. Ellingwood. Oct 85, 16p
Pub. in Jnl. of Structural Engineering III, n10 p2197-2213 Oct 85.

Keywords: *Buildings, *Vibration, Motion, Wind pressure, Loads(Forces), Deflection, Stiffness, Reprints.

Fluctuating wind forces on tall buildings can cause excessive building motion which may be disturbing to the occupants. A method to assess motion sensitivity of square isolated buildings is developed using random vibration theory to relate dynamic along-wind, across-wind, and torsional forces to building accelerations. Wind tunnel test data are analyzed to determine the spectra of force components and correlations among components of force and mechanical coupling of components of motion introduced by eccentricities of the centers of mass and rigidity from the building centroid are examined. Comparisons are made with more common building analyses, where the forces are assumed to be statistically uncorrelated and the components of motion are assumed to be uncoupled.

*600,130*
**PB87-108635** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Wind Tunnel Simulation of Along-Wind Tall Building Response: Micrometeorological and Similarity Considerations.**
Final rept.,
E. Simiu. Jun 78, 1p
Pub. in Colloquium on Industrial Aerodynamics (3rd), Aachen, West Germany, June 18-20, 1978.

Keywords: *Buildings, *Wind pressure, *Towers, Dynamic structural analysis, Simulation, Comparison, *Wind effects, *Tall buildings, Wind tunnel tests, Atmospheric boundary layer.

A discussion is presented of the implications of recent results of atmospheric boundary layer research for the wind tunnel simulation of the along-wind response of tall structures. It is shown, on the basis of similarity considerations and of recently developed models of the atmospheric flow structure, that the turbulent fluctuations which cause resonant amplification effects in tall buildings are not similar in long wind tunnels to the corresponding fluctuations in atmospheric flows. The question is discussed of the corrections that should be applied to the along-wind response measurements obtained in the wind tunnel in order to account for differences between turbulence spectra in the atmosphere and in the laboratory.

## General

*600,131*
**PB86-166105** PC **A07**/MF **A01**
Factory Mutual Research Corp., Norwood, MA.
**Experimental Fires in Multiroom/Corridor Enclosures.**
Final rept.,
G. Heskestad, and J. P. Hill. Jan 86, 132p NBS/GCR-86/502
Contract NB83-NADA-4046
Also pub. as Conseil International du Batiment pour la Recherche l'Etude et la Documentation, Rotterdam (Netherlands) rept. no. CIB/W-14/85/10(USA). Prepared in cooperation with Conseil International du Batiment pour la Recherche l'Etude et la Documentation, Rotterdam (Netherlands). Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Fires, Fire tests, Buildings, Flashpoint, *Fire studies, Fire models.

A series of 60 fire tests have been conducted in an enclosure consisting of a corridor and three attached rooms, one of which served as a burn room. The purpose was to establish validation data for theoretical fire models of multi-room fire situations with particular emphasis on health care facilities. Fire sources were propylene gas burners, producing steady fires at 56 and 522 kW as well as fires growing with the square of time at several growth rates up to a maximum output of 2MW.

*600,132*
**PB86-193166** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Assessing Toxic Hazard as It Relates to Overall Fire Hazard.**
Final rept.,
A. J. Fowell. 1985, 14p
Pub. in Fire Technology 21, n3 p199-212 Aug 85.

Keywords: *Fires, *Buildings, Fire hazards, Toxicity, Combustion products, Furniture, Reprints, Fire models.

A framework is proposed for assessing hazards associated with the spread of smoke and hot gases from fires in buildings, and the current predictive capabilities for each component of that framework are described. Particular attention is given to the significance of the toxicity of the combustion products of a material in relation to its other fire properties.

*600,133*
**PB86-203049** PC **A06**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**'Fireform' - A Computerized Collection of Convenient Fire Safety Computations,**
H. E. Nelson. Apr 86, 101p NBSIR-86/3308
Sponsored by Department of Health and Human Services, Washington, DC., and Air Force Engineering and Services Center, Tyndall AFB, FL.

Keywords: *Fires, *Fire safety, Buildings, Computer programs, Smoke, Fire detection systems, Sprinkler systems, *Fire models, Fire studies.

A computerized system of convenient fire safety computations is presented. Subjects covered include smoke filling in a room, sprinkler/detector activation, smoke flow through (small) openings, temperatures and pressures developed by fires, flashover and fire severity prediction, fire propagation (in special cases), and simple egress estimation. All programs are based on established formulas and are programmed in BASIC for microcomputers.

*600,134*
**PB86-209996** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Data for Room Fire Models.**
Final rept.,
J. A. Rockett. 1984, 15p
Pub. in Jnl. of Combustion Science and Technology 40, n1-4 p137-151 1984.

Keywords: *Fires, *Fire tests, Data, Reprints, *Room fires, Five models.

Data needs for state-of-the-art single room fire models are discussed using several examples. Three types of data are needed: geometric, thermal and chemical. Needed geometric data generally present no problem and are not discussed. Under thermal data those quantities which determine the transient surface temperature of objects in the room are considered.

*600,135*
**PB86-210705** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**ASHRAE (American Society of Heating, Refrigeration and Air-Conditioning Engineers) Design Manual for Smoke Control.**
Final rept.,
J. H. Klote. 1984, 6p
Pub. in Fire Safety Jnl. 7, n1 p93-98 1984.

Keywords: *Smoke, Smoke abatement, Fire safety, Buildings, Reprints.

For many years smoke has been recognized as a major killer in fire situations. In response to the problem, the concept of controlling smoke movement in building fires has developed. The American Society of Heating, Refrigeration, and Air-Conditioning Engineers and the U.S. Veterans Administration have sponsored a design manual for smoke control systems. The paper provides an overview of the manual with emphasis on the principles of smoke control, stairwell pressurization, zone smoke control, and computer analysis.

*600,136*
**PB86-223104** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Federal Building Life-Cycle Cost (FBLCC) Computer Program User's Guide,**
S. R. Petersen. May 86, 91p NBS/TN-1222, NBS/SW/DK-86/007A
Contract DE-AI01-86CE73041
For system on diskette, see PB86-223112. Sponsored by Department of Energy, Washington, DC.

Keywords: *Buildings, National government, Prices, Computation, *Energy conservation, *Life cycle cost, Energy use, FBLCC computer program, User manuals(Computer programs).

The FBLCC Computer Program and the User's Guide provide computational tools and energy price data for performing life-cycle cost (LCC) analyses of Federal buildings and related subsystems. Two kinds of Federal building projects can be evaluated with FBLCC: (1) LCC analysis of projects directly related to energy conservation and renewable energy, and (2) LCC analysis of projects not directly concerned with energy conservation or renewable energy.

*600,137*
**PB86-223112** CP **T99**
National Bureau of Standards, Gaithersburg, MD.
**Federal Building Life-Cycle (FBLCC) Program Diskette.**
Software,
S. R. Petersen, and W. Bethea. May 86, 1 diskette
NBS/SW/DK-86/007
The software is contained on 5 1/4-inch diskette, double sided, double density compatible with the IBM PC microcomputer. Diskettes are in the ASCII format. Price includes documentation, PB86-223104.

Keywords: *Software, *Buildings, National government, Prices, Computation, *Energy conservation, *Life cycle costs, Energy use, Diskettes, L=BASIC, H=IBM PC.

The Federal Building Life-Cycle Cost Program provides computational tools and energy price data for performing life-cycle cost (LCC) analyses of Federal buildings and related subsystems. The methods and procedures used in these LCC analyses are based on rules set forth by the U.S. Department of Energy's Federal Energy Management Program and U.S. Office of Management and Budget. The 5-1/4 inch diskette contains the FBLCC programs and related data files in MD-DOS format. The documentation for the FBLCC program is contained in 'A User's Guide to the Federal Building Life-Cycle Cost (FBLCC) Program,' NBS-TN 1222. ...Software Description: The software is written in the BASIC programming language for implementation on an IBM PC-compatible microcomputer under the MS-DOS operating system. Memory requirement is 64K.

*600,138*
**PB87-106019** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Design of Effective Water Spray Cooling in Stairwell-Sprinkler Systems.**
Final rept.,
L. Y. Cooper. 1981, 15p
Sponsored by Department of Labor, Washington, DC., and Department of Health and Human Services, Washington, DC.
Pub. in Proceedings of Engineering Applications of Fire Technology Workshop, Gaithersburg, MD., April 16-18, 1980, p89-103 1981.

Keywords: *Sprinkler systems, *Fire safety, Cooling, Stairwells.

The potential benefits of sprinkler protection of open stairways during fires are discussed. One of these benefits results from the cooling of products of combustion which pass through the stairwell penetration. An example scenario is introduced to illustrate this benefit. A relevant experimental study of the performance of stairwell-sprinkler systems is summarized. The results of the study are used to develop a guide for the design of stairwell-sprinkler systems with an objective of efficient evaporative cooling of flow through fire gases. Examples on the use of these design guides are presented.

*600,139*
**PB87-113700** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Determination of Energy Reduction in Retrofitted Homes.**
Final rept.,
Y. M. Chang, and R. A. Grot. 1984, 1p
Pub. in ASHRAE Jnl. (American Society of Heating, Refrigeration and Air-Conditioning Engineers) 26, n5 p39 1984.

Keywords: *Houses, *Weatherproofing, *Energy conservation, Low income housing, Demonstration projects, Case studies.

The report presents a technique for analyzing the effect of energy saving retrofits installed in low-income housing under a nationwide weatherization demonstration program. A tracking technique based on the calculated balance-point temperature of each home prior to the weatherization, was developed to predict the would-be fuel consumption over a period of time as if the house were not weatherized. Fuel reduction is reported for more than 100 homes using different fuels in seven cities across the nation, selected to represent various climate zones and geographical locations. It was found that the average saving in fuel consumption for dwellings in each city is about 30 percent.

*600,140*
**PB87-113718** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Reference Building - One Approach in the Evolution of Building Energy Performance Criteria for Houses.**
Final rept.,
J. L. Heldenbrand, and S. R. Petersen. 1982, 13p
Sponsored by Department of Energy, Washington, DC.
Pub. in ASHRAE Transactions, v88 pt1 p387-399 1982.

Keywords: *Houses, *Energy, Performance, Criteria.

No abstract available.

*600,141*
**PB87-120200** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Smoke Control and Fire Evacuation by Elevators.**
Final rept.,
J. H. Klote, and G. Tamura. 1986, 15p
Pub. in American Society of Heating, Refrigerating and Air-Conditioning Engineers Transactions 92, Pt 1A p231-245 1986.

Keywords: *Elevators(Lifts), Stairways, Reprints, *Evacuation, *Building fires, *Smoke control, Control systems.

In recent years, the possibility of using elevators as a means of fire escape has received considerable attention. The interest has been sparked by an increased awareness of life safety problems of the handicapped and also general fire evacuation problems of high-rise buildings. The use of elevators as a means of fire evacuation is a potential solution to the problem. The major technical obstacle to this is smoke contamination of elevator lobbies and shafts. The paper discusses elevator smoke control systems including criteria for evaluation and presents an analysis of airflow due to elevator car motion. Computer analysis of several elevator smoke control systems are included for several combinations of open and closed doors and for summer and winter conditions.

*600,142*
**PB87-122362** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Chimney Fires: Intensity and Duration.**
Final rept.,
R. D. Peacock. 1986, 17p
Sponsored by Consumer Product Safety Commission, Washington, DC., and Department of Energy, Washington, DC.
Pub. in Fire Technology 22, n3 p234-252 Aug 86.

Keywords: Fire safety, Stoves, Creosote, Fireplaces, Reprints, *Chimney fires, Wood burning appliances.

A series of tests was conducted in five instrumented chimneys to study the intensity and duration of chimney fires due to the ignition and burning of combustible deposits accumulated on chimney linings over a prolonged period of time. These tests were conducted: (1) to establish typical conditions including temperatures in the chimneys and on combustible surfaces nearby, and (2) to determine the duration of the burnout as evidenced by elevated temperatures within the chimney. The results of these tests point out some areas where the codes and standards covering residential wood heating appliances should be updated to better protect against failure due to chimney fires.

*600,143*
**PB87-128088** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

**NBS (National Bureau of Standards)/Harvard Mark 6 Multi-Room Fire Simulation.**
Final rept.,
J. A. Rockett, and M. Morita. 1985, 15p
Pub. in Fire Science Technology 5, n2 p149-163 1985.

Keywords: *Fires, *Computerized simulation, Mathematical models, Reprints, *Building fires, FORTRAN 77 programming language.

The NBS/HARVARD Mark VI multi-room fire simulation program structure is discussed and compared with Harvard V. In addition to the current, operating version of VI, a development version is being used to test enrichments which can be readily moved into the operational version as they mature. The program is written in ANSI standard FORTRAN 77 and is transportable to computers of various manufacture.

*600,144*
**PB87-134300** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Fire Safety Evaluation System for NASA (National Aeronautics and Space Administration) Office/ Laboratory Buildings,**
H. E. Nelson. Nov 86, 38p NBSIR-86/3404
Sponsored by National Aeronautics and Space Administration, Washington, DC.

Keywords: *Fire safety, Laboratories, Office buildings, Evaluation, NASA, Risk assessment.

A fire safety evaluation system for office/laboratory buildings is developed. The system is a life safety grading system. The system scores building construction, hazardous areas, vertical openings, sprinklers, detectors, alarms, interior finish, smoke control, exit systems, compartmentation, and emergency preparedness.

*600,145*
**PB87-140182** PC **A03**/MF **A01**
Factory Mutual Research Corp., Norwood, MA.
**Calculated Interaction of Water Droplet Sprays with Fire Plumes in Compartments.**
Final rept.,
R. L. Alpert, and M. M. Delichatsios. Dec 86, 48p NBS/GCR-86/520
Contract NB83-NADA-4014
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: Computerized simulation, Drops(Liquids), Ceilings(Architecture), Gas flow, Plumes, *Building fires, *Fire suppression, Water sprays, Compartments.

The objective of the program is to analyze mathematically, through the use of computer solutions, the complex interaction between water droplet sprays and the buoyancy-driven gas flows induced by a building fire. The specific goal is to obtain scientific correlations relating spray penetration through the fire plume and cooling of the fire environment to a set of controlling parameters such as fire intensity, spray characteristics and geometric factors (i.e. compartment size or ceiling height). Such correlations could then be used in current zone models of compartment fires.

*600,146*
**PB87-140216** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Building Technology Project Summaries 1986,**
R. N. Wright. Dec 86, 68p NBSIR-86/3490
See also PB85-240448.

Keywords: Construction, Bibliographies, Technology, Projects, Abstracts, Buildings, Loads(Forces), Reliability, Thermal analysis, Thermal measurements, Acoustics, Illuminating, Plumbing, Construction materials, Roofing, Concretes, Refrigerants, *Building technology, Earthquake engineering, Solar equipment.

The Center for Building Technology (CBT) of the National Bureau of Standards (NBS) is the national building research laboratory. It works cooperatively with other organizations, private and public, to improve building practices. It conducts laboratory, field, and analytical research. It develops technologies to predict, measure, and test the performance of building materials, components, systems, and practices. This knowledge is required for responsible and cost-effective decisions in the building process and cannot be obtained through proprietary research and development. CBT provides technologies needed by the building community to achieve the benefits of advanced computation and automation. CBT does not promulgate building standards or regulations, but its technologies are widely used in the building industry and adopted by governmental and private organizations that have standards and codes responsibilities. The report summarizes the projects underway in the Center during 1986.

# BUSINESS & ECONOMICS

## Consumer Affairs

*600,147*
**PB87-103248** PC **A09**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Uniform Laws and Regulations as Adopted by the National Conference on Weights and Measures (71st), 1986.**
Final rept.,
S. Brickenkamp. Sep 86, 185p NBS/HB-130-1987
Supersedes PB86-115672. Also available from Supt. of Docs as SN003-003-02754-5.

Keywords: *Weight measurement, *Regulations, Standardization, Handbooks, Units of measurement, Packaging, Labels, Consumer affairs, Prices, Sales, National Bureau of Standards, *Weights and measures, Open dating.

The handbook, revised annually, compiles the uniform laws and regulations developed by the Committee on Laws and Regulations of the National Conference on Weights and Measures (NCWM). The compilation itself was approved by the NCWM in 1979, and this edition includes amendments adopted by the Conference at its annual meeting in 1986. The title of the handbook and the titles of the laws and regulations compiled in it were changed at the 1983 annual meeting of the NCWM. A new index for the entire handbook has been added to this year's edition.

*600,148*
**PB87-140588** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**DOE/NBS (Department of Energy/National Bureau of Standards) Forum on Testing and Rating Procedures for Consumer Products, October 2-3, 1985.**
Final rept.,
R. D. Dikkers. Jul 86, 68p NBSIR-86/3412
DE-AI01-86CE23842
Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.

Keywords: Meetings, Consumer affairs, Tests, Heat pumps, Air conditioners, Furnaces, Boilers, Refrigerators, Heating equipment, Water heaters, *Consumer products.

One hundred thirty-four persons participated in a Forum on Testing and Rating Procedures for Consumer Products held at the National Bureau of Standards (NBS), Gaithersburg, Maryland, on October 2-3, 1985. The objectives of the forum, which was planned in cooperation with various industry associations, were: (1) to provide a line of communication between test procedure users and test procedure developers; (2) to provide an opportunity for participants to present technical and research issues concerning Department of Energy (DOE) test procedures that need to be addressed; and (3) to assist DOE and NBS in establishing a future agenda for the development and/or revision of testing and rating procedures. The report summarizes discussions, conclusions and recommendations developed by the forum participants for the following consumer products: heat pumps and air conditioners; furnaces, boilers, and household heaters; water heaters; refrigerators, refrigerator-freezers and freezers.

## International Commerce, Marketing, & Economics

*600,149*
**PB86-186715** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**Standards and the Economy Worldwide.**
Final rept.,
W. G. Leight. 1986, 4p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 14, n1 p47-50 Jan 86.

Keywords: *Standards, *International trade, Developing countries, Reprints, *Product standards, *Engineering standards, *World trade markets, *Third World countries, Trade, Economy.

Product and engineering standards play a vital role in technological progress, especially for developing countries. Aid to less-developed nations may lead to better trade opportunities to the mutual benefit of both parties. Accordingly, many groups pursue programs to foster Third World development at the same time that the standards community promotes the widespread use and adoption of high quality domestic standards. The paper describes efforts at the National Bureau of Standards to relate U.S. standards activities to the needs of developing countries and to draw attention to corresponding programs at ASTM.

*600,150*
**PB86-213675** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**GATT (General Agreement on Tariffs and Trade) Standards Code Activities of the National Bureau of Standards 1985,**
Annual rept.,
J. R. Overman. Apr 86, 39p NBSIR-86/3376

Keywords: *Standards, *International trade, Technical assistance, Regulations, US NBS, General Agreement on Tariffs and Trade, GATT standards, Foreign.

The report describes the GATT Standards Code activities conducted by the Standards Code and Information program, National Bureau of Standards (NBS), for calendar year 1985. NBS responsibilities include operating the U.S. GATT inquiry point for information on standards and certification activities; notifying the GATT Secretariat of proposed U.S. Federal government standards-based rules that might significantly affect trade; assisting U.S. industry with standards-related trade problems; and responding to inquiries about proposed foreign and U.S. regulations.

*600,151*
**PB87-122222** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**Making Effective Use of ISONET and GATT Enquiry Points.**
Final rept.,
W. G. Leight. 1986, 9p
Pub. in Proceedings of Triennial IFAN Conference (5th), Annual SES Conference (35th), Applying the World's Standards, Philadelphia, PA., September 28-October 1, 1986, p1-9.

Keywords: *Standards, *Information systems, *International trade, Barriers, Subject indexing, Efficiency, Effectiveness, *Certification, *Trade, References(Standards), National Bureau of Standards, GATT system, ISONET system.

The National Center for Standards and Certification Information (NCSCI) at the National Bureau of Standards provides the Enquiry Points for both ISONET and GATT. The paper discusses the nature, scope, and size of the NCSCI reference collection and the services offered to domestic and foreign contacts. Based on the generic nature of search for information and NCSCI experience in attempting to provide efficient and effective responses to inquiries, several problem areas are identified. The proposed solutions will require the coordinated efforts of producers, conveyors, and users of standards and the information pertaining to them.

# CHEMISTRY

## Analytical Chemistry

*600,152*
**AD-A170 328/9** PC A02/MF A01
National Bureau of Standards, Gaithersburg, MD.
**New Techniques and Opportunities in High Temperature Mass Spectrometry,**
John W. Hastie. 1984, 19p ARO-18375.2-CH
Contract MIPR-102-84
Pub. in Pure and Applied Chemistry, v56 p1583-1600 1984.

Keywords: *Mass spectrometry, Laboratory procedures, High temperature, Flames, Molecular beams, Laser pumping, Electron impact spectra, Ionization, Cross sections, Thermal properties, Reprints, Knudsen effusion, LIVMS(Laser Induced Vaporization Mass Spectrometry).

In the present discussion, emphasis is given to recent developments and remaining problems in the application of mass spectrometry to high temperature materials chemistry. Examples of application areas discussed include: Knudsen effusion mass spectrometry of gas-solid reactions, with equilibrium or kinetic control; high-pressure molecular beam sampling mass spectrometry of flames and laser-vapor-plumes, and transpiration mass spectrometry of gas-liquid-solid and ceramic-slag-salt systems. Certain maxims are examined, including use of ionization cross-section approximations. Evidence of departure from the key assumption of a temperature-independent electron impact process is given, including temperature-dependent parent-ion fragmentation and cross section behavior. Errors arising from the use of cross section additivity and electron energy-scaling approximations are also examined.

*600,153*
**PB86-160082** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Determination of Nanogram Quantities of Vanadium in Biological Material by Isotope Dilution Thermal Ionization Mass Spectrometry with Ion Counting Detection.**
Final rept.,
J. D. Fassett, and H. M. Kingston. 1985, 5p
Pub. in Analytical Chemistry 57, n13, p2474-2478 Nov 85.

Keywords: *Vanadium, *Trace elements, *Bioassay, Isotopic labeling, Concentration(Composition), Chemical analysis, Mass spectroscopy, Separated, Leaves(Botany), Liver, Oysters, Tissue(Biology), Blood analysis, Reprints, *Biological processes, *Isotope dilution thermal ionization mass spectroscopy, Standard reference materials, Procedures.

A procedure has been developed for the determination of nanogram quantities of vanadium in biological matrices by isotope dilution mass spectrometry that uses a 50V spike enriched to 64 atom %. The V is chemically purified by a Chelex-100 separation and loaded onto a carburized Re filament. The procedure has been applied to the determination of V in various NBS Standard Reference Materials: Oyster Tissue, SRM 1566; Citrus Leaves, SRM 1572; Bovine Liver, SRM 1577a; and Human Serum, SRM 909. The certified concentration of V in the Human Serum SRM is the lowest of any Standard Reference Material.

*600,154*
**PB86-162070** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Solid-State 13C NMR Determination of Methyltin(IV) Structure. Crystal and Molecular Structure of Dimethyltin(IV) Bis(1-Pyrrolidinecarbodithiate).**
Final rept.,
T. P. Lockhart, W. F. Manders, and E. O. Schlemper. 1985, 3p
Pub. in Jnl. of the American Chemical Society 107, n25 p7451-7453 1985.

Keywords: *Nuclear magnetic resonance, *Quantitative chemical analysis, Organometallic compounds, Reprints, *Methyltin.

Solid-state 13C NMR and X-ray crystallographic studies of the title compound, Me2Sn(S2CN(CH2)4)2, are reported. The magnitude of 1J(119Sn,13C), (1J), measured for a polycrystalline sample, is 705 Hz. When a previously described relationship between (1J) and the Me-Sn-Me angle was used, an angle of 138.6 degrees was predicted for the molecule. The discrepancy between the result and the published X-ray structure (Me-Sn-Me angle = 130 (2) degrees) led to a redetermination of the crystal structure by X-ray. Solution of the structure of the orthorhombic crystals in the Pmmn space group yielded a chemically reasonable structure (R=0.029, Rw=0.038) in which the pyrrolidine carbons C3 and C4 are disordered across the mirror plane at y=1/4. Similar to other dimethyltin(IV) bis(dithiocarbamates), Me2Sn(S2CN(CH2)4)2 adopts a distorted octahedral geometry: the Me-Sn-Me angle is 137.3(3), and the dithiocarbamate ligands are coplanar with tin but adopt an anisobidentate coordination geometry (Sn-S=2.518, 2.938 Angstroms). The presence of two mirror planes results in a simple solid-state 13C NMR spectrum. In contrast to the accurate NMR-derived prediction, published Mossbauer data led to a predicted Me-Sn-Me angle (123.5 degrees) 14 degrees in error.

*600,155*
**PB86-163409** PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Literature Review of the Chemical Nature and Toxicity of the Decomposition Products of Polyethylenes,**
M. Paabo, and B. C. Levin. Jan 86, 68p NBSIR-85/3268
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Combustion products, *Polyethylene, *Toxicology, Pyrolysis, Literature surveys.

The literature on polyethylenes has been reviewed with an emphasis on the identification of gaseous products generated under various thermal decomposition conditions and the toxicity of those products. The review is limited to publications in English through 1984. The analytical chemical studies of the thermal decomposition products generated under vacuum, inert and oxidative experimental conditions are described. In oxidative atmospheres, which most closely simulate real fire conditions, carbon monoxide (CO) was found to be the predominant toxicant. Acrolein was another toxicant often noted in these reviewed studies. More acrolein was generated under non-flaming than under flaming conditions. Results from seven different test procedures were considered in assessing the acute inhalation toxicity of combustion products from various polyethylene formulation. The combustion products generated from the polyethylenes studied in the non-flaming mode appeared to be slightly more toxic than those produced in the flaming mode.

*600,156*
**PB86-178902** PC A09/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Technical Activities 1985, Center for Analytical Chemistry,**
R. A. Durst, H. S. Hertz, and J. K. Taylor. Dec 85, 188p NBSIR-85/3272
See also PB85-164952.

Keywords: *Chemical analysis, *Standards, *Research projects, Inorganic compounds, Organic compounds, Particles, Gases.

The report summarizes the technical activities of the Center for Analytical Chemistry at the National Bureau of Standards. It emphasizes activities over the Fiscal Year 1985 in the Inorganic Analytical Research Division, the Organic Analytical Research Division, and the Gas and Particulate Science Division. In addition, it describes certain special activities in the Center including quality assurance and voluntary standardization coordination.

*600,157*
**PB86-185477** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Materials Div.
**Graphite Furnace Atomic Absorption Spectrophotometers as Automated Element-Specific Detectors for High-Pressure Liquid Chromatography. The Determination of Arsenite, Arsenate, Methylarsonic Acid and Dimethylarsinic Acid.**
Final rept.,
F. E. Brinckman, K. L. Jewett, W. P. Iverson, K. J. Irgolic, and K. C. Ehrhardt. 1980, 16p
Sponsored by Environmental Protection Agency, Washington, DC.
Pub. in Jnl. of Chromatography 191, p31-46 1980.

Keywords: *Chromatographic analysis, *Arsenates, Chemical analysis, Arsenic organic compounds, Arsenic organic acids, Reprints, *Arsenites, *Arsonic acid/methyl, *Arsine oxide/dimethyl-hydroxy, High pressure liquid chromatography.

Techniques for the determination of trace element compounds at ppb and ppm levels (in contrast to the determination of the total element concentration) are a prerequisite for the study of the transformations of trace elements in biological systems and the interactions of trace element compounds with biologically important molecules. Two automated high-pressure liquid chromatography (HPLC) systems with element-specific detectors, capable of detecting, identifying and quantitating trace element compounds were developed independently in our laboratories. One of the detectors consists of a Perkin-Elmer graphite furnace atomic absorption spectrometer (GFAA) and a specially adapted autosampler, whereas a Hitachi-Zeeman GFAA, a sample valve, an injector and associated electronics to control the analysis sequence comprise the components of the other detector. The capability of these systems to speciate trace element compounds is demonstrated using arsenite, arsenate, methylarsonic acid (MAA) and dimethylarsinic acid (DMAA) as examples. The separation schemes developed for the four arsenic compounds were used to speciate these compounds in soil extracts and drinking waters. The separation efficiency achieved thus far can very likely be improved through development of better column materials and mobile phases. The work with arsenic compounds clearly shows the great potential of these HPLC-GFAA analytical systems in the area of environmental trace element chemistry, in the field of physiological chemistry and in trace element-related nutritional studies.

*600,158*
**PB86-187028** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Laser-Enhanced Ionization Spectrometry for Trace Metal Analysis.**
Final rept.,
G. C. Turk, J. C. Travis, and J. R. DeVoe. c1983, 9p
Pub. in Jnl. de Physique, Colloque C7, p301-309 1983.

Keywords: *Chemical analysis, *Trace elements, Metals, Reprints, Laser spectroscopy, Flame spectroscopy.

Laser-enhanced ionization spectrometry is an application of optogalvanic spectroscopy for quantitative analysis of trace concentrations of metallic elements in flames. The paper reviews the scientific literature on the subject, and summarizes the performance of the method in its present state of development.

*600,159*
**PB86-187689** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**High Resolution CPMAS 13C NMR of Organometallic Solids. Observations of 'J' Coupling to Tin.**
Final rept.,
W. F. Manders, and T. P. Lockhart. 1985, 5p
Pub. in Jnl. of Organometallic Chemistry 297, p143-147 1985.

Keywords: *Tin organic compounds, Organometallic compounds, Nuclear magnetic resonance, Reprints, *Stannanes/methyl, Coupling constants, Chemical shifts, Carbon 13.

Chemical shift and (sup 1)J (117,119)Sn (13)C data from cross polarization magic angle spinning (CPMAS) proton-decoupled solid-state (13)C NMR experiments are given for the methyltin carbon in (Me2SnS)3, Me3SnOAc, Me2Sn(acetylacetonate)2, Me2SnC(1)2(dimethylsulfoxide), and amorphous (Me2SnO)n. The relationship between the magnitude of the coupling constant and the coordination at tin is

examined by reference to X-ray structure data. The tin-methyl (13)C chemical shift was sensitive to slight variations in bond angles and bond lengths. The presence of isotopically abundant NMR-active nuclei in the molecule broadens lines, and can prevent resolution of the J coupled interaction.

*600,160*
**PB86-190717** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Determination of Trace-Level Chromium(VI) in the Presence of Chromium(III) and Iron(III) by Flow Injection Amperometry.**
Final rept.,
K. W. Pratt, and W. F. Koch. 1986, 4p
Pub. in Analytical Chemistry 58, n1 p124-127 Jan 86.

Keywords: *Chromium, *Iron, Speciation, Voltammetry, Reprints, *Amperometry, Flow injection.

Chromium(VI) is determined by flow injection amperometry at Au and Iodized Pd electrodes without prior chromatographic or other separation. Dissolved O2 and Cr(III) do not interfere. Use of H3PO4 as the supporting electrolyte suppresses the interference from Fe(III). Chloride ion interferes in the determination at Au electrodes but not at Pd electrodes. Decay in sensitivity of the electrodes with time has been eliminated by continuous preconditioning of the electrode with a pulsed-potential wave form in place of constant-potential amperometry. The detection limit for Cr(VI) is 5 ng/mL.

*600,161*
**PB86-192119** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Optimization of Selectivity Using Sequentially Coupled Capillary Columns.**
Final rept.,
H. T. Mayfield, and S. N. Chesler. 1985, 7p
Pub. in High Resolution Chromotography and Chromatography Communications 8, p595-601 Sep 85.

Keywords: *Chromatography, Reprints, Selectivity.

The investigation lays groundwork for the development of an optimization system for sequentially coupled capillary column systems. Three methods for calculating effective capacity factors were obtained from the literature and were tested to determine suitability for optimization use, using four test analytes and two dissimilar columns. The work concentrates on the development of a method for the estimation of optimum column temperatures in sequentially coupled systems.

*600,162*
**PB86-192994** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Observations on the Determination of Phi(rho z) Curves for Thin Films in the Analytical Electron Microscope.**
Final rept.,
D. E. Newbury, R. L. Myklebust, A. D. Romig, and K. W. Bieg. 1983, 3p
Pub. in Microbeam Anal. 18, p168-170 1983.

Keywords: *Electron microscopy, Thin films, Chemical analysis, Microanalysis, Gold foil, Depth, Distribution functions, X ray spectroscopy, Reprints, Electron trajectories, Microbeams, *Energy dispersive x ray spectroscopy.

The depth distribution of x-ray production in thin gold foils generated by a 100 keV electron beam has been studied by Monte Carlo electron trajectory simulation and binary thin foil experiments. For foils tilted at 45 degrees to the beam, the depth distribution function is strongly peaked for foils greater in thickness than 100 nm. Because of significant backscattering, binary foils with the tracor placed on the foil bottom do not yield an accurate depth distribution function.

*600,163*
**PB86-193232** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Laser Microprobe Mass Spectrometry.**
Final rept.,
D. S. Simons. 1984, 6p
Pub. in Springer Ser. Chem. Phys. 36, nSIMS 4 p158-163 1984.

Keywords: *Mass spectroscopy, Reprints, *Laser microprobe analysis.

Laser microprobe mass spectrometry has been applied to a wide variety of problems in chemistry, biology, and materials science. The concept of the instrument is described, analytical features are discussed and several illustrative applications are presented.

*600,164*
**PB86-193257** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Analytical Standards for the Analysis of Chrysotile Asbestos in Ambient Environments.**
Final rept.,
J. A. Small, E. B. Steel, and P. J. Sheridan. 1985, 5p
Sponsored by Environmental Protection Agency, Research Triangle Park, NC.
Pub. in Analytical Chemistry 57, n1 p204-208 1985.

Keywords: *Asbestos, *Standards, Chemical analysis, Reprints, Transmission electron microscopy, *Chrysotile.

Results of a program for the development of standard materials for the analysis of chrysotile asbestos in nonworkplace environments are presented. These standards consist of carbon-coated Nucleport filter sections which contain predictable loadings of chrysotile asbestos fibers mixed with an urban air particulate matrix so that they resemble field samples. One standard contains an ambient loading, approximately 9 asbestos fibers/0.01 square millimeter of filter. Because of the low fiber counts and large standard deviation in the average fiber loading, the standard does not have a certified value for the fiber loading. Instead the results are presented in an analysis report. The second standard contains a slightly higher loading of asbestos, approximately 30 fibers/0.01 square millimeter of filter. The standard includes a certified fiber loading with the uncertainty in the value expressed as a 95/95 tolerance interval about a five-count mean.

*600,165*
**PB86-193265** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Fabrication of Metals and Metal Alloys as Particle Standards.**
Final rept.,
J. A. Small, J. A. Norris, and R. L. McKenzie. 1983, 2p
Pub. in Microbeam Anal. 18, p209-210 1983.

Keywords: *Particle size, *Microanalysis, Chemical analysis, Metals, Reprints, *Calibration standards.

Recently, in studying the mechanism of analyte excitation in spectro-chemical analysis it was noticed that the spark of the emission spectrometer very efficiently produced particles in the 5 nanometers-10 micrometers size range. These particles may be suitable to serve as standards which could provide a large number of pure metal or metal alloy particles in a broad size range. Since the particles can be produced in large numbers, they can be used as particle standards for both micro and bulk analytical techniques.

*600,166*
**PB86-193935** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Studies of Physical Mechanisms in Laser-Enhanced Ionization in Flames.**
Final rept.,
P. K. Schenck, J. C. Travis, and G. C. Turk. 1983, 10p
Sponsored by Centre National de la Recherche Scientifique, Paris (France).
Pub. in J. Phys. Colloq., nC7 p75-84 1983.

Keywords: Reprints, *Laser enhanced ionization, *Flame spectroscopy, Atomic spectroscopy.

Laser enhanced ionization (LEI) mechanisms which result in locally large neutral atom depletions in flames are discussed. In addition, this results in a locally large perturbation of the ionization rate of the flame which can be observed by an imaging technique. Two theoretical models of the physical motion of the LEI electrons and ions in the flame and their applicability to experimental observations are discussed.

*600,167*
**PB86-195575** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Rising Interest in Quality Assurance.**
Final rept.,
J. K. Taylor. 1984, 1p
Pub. in Trac-Trends in Analytical Chemistry 3, n4 p2 1984.

Keywords: *Quality assurance, Chemical analysis, Statistical analysis, Reprints, Standard reference materials.

There is an increasing awareness that data quality is enhanced if the data are produced by a measurement system in a state of statistical control. The basic elements of a quality assurance program to attain the objective are described, and the expected benefits are summarized.

*600,168*
**PB86-195807** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Lithium-Activated Silicon Detector-Specimen Angles in an AEM (Analytical Electron Microscopy).**
Final rept.,
R. L. Myklebust. 1983, 3p
Pub. in Microbeam Anal. 18, p174-176 1983.

Keywords: *Electron microscopy, Trajectories, Simulations, Detectors, X rays, Quantitative analysis, Reprints.

For quantitative energy dispersive analysis in an AEM, the position of the detector with respect to the specimen and electron beam must be known. The angle of the detector with respect to the electron beam is generally a fixed instrumental parameter that is known for each system. The specimen tilt axis is also an easily obtained parameter for each microscope and the azimuthal angle of the detector with respect to the specimen tilt axis can be specified. The angle between the detector and the specimen surface (usually called the take-off-angle) can be easily determined if the specimen is tilted toward the detector (azimuthal angle = 90 degrees, detector axis at right angles to the tilt axis). However, in many instruments, this is not the case and calculating the take-off-angle is more complicated. In the following discussion, the angular relations between the detector and the axes of the specimen together with the take-off-angle are derived.

*600,169*
**PB86-195997** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Post Column Solvent Trapping Technique for the Analysis of Very Volatile Halocarbons.**
Final rept.,
F. R. Guenther, and S. N. Chesler. 1983, 2p
Pub. in HRC amp CC, Jnl. of High Resolution Chromatography and Chromatography Communications 6, n12 p684-685 1983.

Keywords: *Aluminum oxide, *Gas chromatography, Halohydrocarbons, Reprints, *Water pollution detection, Post column trap.

A capillary gas chromatographic method is described by which volatile halocarbon analytes eluting under a methanol or water solvent peak can be analyzed. The method consists of injecting the analytes onto a thick film SE-52 capillary column. The exit end of the column enters a post column trap packed with activated alumina. The trap selectively adsorbes the methanol solvent, allowing the analytes to pass to the detector unhindered. Data is presented which show a standard deviation in the response factors relative to the vinyl chloride internal standard of less than 5%. A detection limit of 1 ug/mL chloromethane is estimated.

*600,170*
**PB86-196037** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Rate of Calcium Hydroxide Precipitation Measured by Electrical Conductance.**
Final rept.,
P. W. Brown, K. Galuk, and G. Frohnsdorff. 1984, 4p
Pub. in Jnl. Cement and Concrete Research 14, n6 p843-846 1984.

Keywords: *Calcium hydroxide, *Precipitation, *Calorimetry, Conductance, Seeding, Reprints, Induction period.

The rates of calcium hydroxide precipitation from supersaturated solutions were measured. Precipitation rates were observed to depend on whether the solutions were seeded with Ca(OH)2 or with C-S-H, or were unseeded. Calorimetric measurements indicated the presence of solid Ca(OH)2 to be ineffectual in promoting the onset of the acceleratory period of C3S hydration. The suggests that Ca(OH)2 precipitation is not the rate determining phenomenon in the regard.

*600,171*
**PB86-196458** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Trace Metal Analysis by Laser-Enhanced Ionization in Flames.**
Final rept.,
J. C. Travis, G. C. Turk, and J. R. DeVoe. 1983, 4p
Pub. in Clinical Chemistry 29, n9 p1683-1686 1983.

Keywords: *Chemical analysis, *Trace elements, Metals, Reprints, Laser spectroscopy, Atomic absorption flame spectroscopy.

A review is given of the atomic flame spectrometric method based on the selective laser-enhancement of atomic ionization rates. A discussion of basic principles, prior literature, and instrumentation is followed by an overview of analytical figures of merit for the method, and a look at the present status and future development areas of the method.

*600,172*
**PB86-196847** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Analytical Formula for Direction Cosines of the Eckart Frame of a Planar Molecule.**
Final rept.,
G. A. Natanson. 15 Nov 85, 4p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Chemical Physics Letters 121, n4-5 p343-346, 15 Nov 85.

Keywords: Reprints, *Eckart frame, *Planar molecule.

An analytical formula is suggested for calculating direction cosines of the Eckart frame of a planar molecule. As one application of the formula, we give a simple way to find the matrix switching of the geometrical body-fixed axes of the formaldehyde molecule to axes of its Eckart frame.

*600,173*
**PB86-199064** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Determination of Sulfur as Arsenic Monosulfide Ion by Isotope Dilution Thermal Ionization Mass Spectrometry.**
Final rept.,
P. J. Paulsen, and W. R. Kelly. 1984, 6p
Pub. in Analytical Chemistry 56, n4 p708-713 1984.

Keywords: *Sulfur, Chemical analysis, Labeled substances, Iron alloys, Sepaation, Reprints, Arsenic sulfides, *Isotope dilution techniques, Thermal ionization mass spectroscopy, Sulfur 32, Sulfur 34, Copper base alloys.

A new procedure has been developed for the determination of microgram quantities of sulfur in metals by isotope dilution thermal ionization mass spectrometry. Typically 1 g metal samples are spiked with (34)S enriched spike, dissolved in a closed system to prevent loss of volatile S compounds using a mixture of HCl/HNO3 acids which oxidizes all S to sulfate. The S is reduced to H2S which is converted to As2S3. The As2S3 is dissolved in an As (+3) - NH3 solution to yield a As/S atom ratio of two. A small portion of this solution equivalent to 1.5 micrograms S is placed on a Re-flat filament with silica gel and the (32)S/(34)S ratio is measured at 950 deg C as the thermally produced (75)As(32)S(+1) and 75AsS+ molecular ion. The ionization efficiency is about 0.1% and the precision of the (32)S/(34)S ratio is typically 0.1% (1s). This procedure has been applied to the determination of S in 11 Cu base and Fe base alloys ranging in S concentration from 2.8 to 80 ppm. At these S levels the chemical blank is the major source of uncertainty. The total uncertainties for these two materials were 0.2 and 1 ppm, respectively.

*600,174*
**PB86-199072** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Analytical Algorithm for Calculation of Spectral Distributions of X-ray Tubes for Quantitative X-ray Fluorescence Analysis.**
Final rept.,
P. A. Pella, L. Feng, and J. A. Small. 1985, 11p
Pub. in X-ray Spectrometry 14, n3 p125-135 1985.

Keywords: *X ray fluorescence analysis, *X ray tubes, Spectrum analysis, Algorithms, Spectral lines, Reprints.

Fundamental parameter methods for quantitative x-ray fluorescence analysis require knowledge of the spectral distributions of x-ray tubes used for sample excitation. The theoretical models for calculation of the spectral distributions include a number of parameters which are not known with sufficient accuracy. Spectral distributions have been measured for just a few x-ray tubes operated at 45-50 kV. The authors have developed an algorithm to calculate x-ray tube spectral distributions by utilizing extensive electron microprobe data obtained under various operating conditions with a Si(Li) detector. The algorithm includes the calculation of the continuum and the ratio of the characteristic line(s) to the underlying continuum intensity at the wavelength of the characteristic line(s).

*600,175*
**PB86-200441** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**On-Line Multidimensional Chromatography Using Supercritical Carbon Dioxide.**
Final rept.,
R. G. Christensen. Dec 85, 5p
Pub. in Jnl. of High Resolution Chromatography and Chromatography Communications 8, p824-828 Dec 85.

Keywords: *Chromatographic analysis, *Aromatic polycylic hydrocarbons, Carbon dioxide, Coal tar, Gas flow, Reprints, *Supercritical flow, High resolution, Two dimensional.

A two-dimensional chromatographic separation is described which makes use of the unusual properties of supercritical carbon dioxide mobile phase. The solvent has the property of giving a separation of polycyclic aromatic hydrocarbons (PAH) on amine-bonded columns similar to that given by usual normalphase solvents, and on octadecylsilane-bonded columns similar to that given by usual reversed-phase solvents. Separations from fractions containing 16 and 18 aromatic carbon atoms are shown.

*600,176*
**PB86-201829** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Measurement of the Oxygen and Carbon Content of Silicon Wafers by Fourier Transform IR (Infrared) Spectrophotometry.**
Final rept.,
A. Baghdadi. 1986, 22p
Pub. in Proceedings of the ACS (American Chemical Society) Symposium Series 295 - Microelectronics Processing: Inorganic Materials Characterization, St. Louis, MO., April 8-13, 1984, p208-229 1986.

Keywords: *Silicon, *Carbon, *Oxygen, Semiconductors(Materials), Infrared spectroscopy, Microelectronics, Fourier transform spectroscopy.

Fourier transform infrared (FT-IR) spectrophotometry is a rapid, nondestructive characterization technique which is being increasingly applied on a large scale to the routine measurement of the oxygen and carbon content of silicon wafers used for the fabrication of microelectronic devices. Control of the oxygen content is needed to achieve acceptable yields in modern device processing, particularly for those processes which utilize oxide precipitates to protect active regions of devices from contamination by metallic impurities during high-temperature processing. The interlaboratory reproducibility of the measurement is not adequate considering the degree of control of the oxygen that is required. This review focuses primarily on the measurement of oxygen and carbon in silicon and on methods for improving quantitative FT-IR absorption measurements on semiconductor wafers.

*600,177*
**PB86-202033** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Performance Appraisal Studies of Laser-Enhanced Ionization in Flames - The Determination of Nickel in Petroleum Products.**
Final rept.,
G. C. Turk, G. J. Havrilla, J. D. Webb, and A. R. Forster. 1984, 5p
Sponsored by Oak Ridge National Lab., TN. Analytical Chemistry Div.
Pub. in Proceedings of the Conference on Analytical Chemistry in Energy Technology (26th), Knoxville, TN., October 11-13, 1983, v19 p63-67 1984.

Keywords: *Nickel, *Petroleum products, Chemical analysis, Laser enhanced ionization, Tunable lasers.

Laser-enhanced ionization (LEI) in flames is an ultrasensitive atomic flame spectrometric technique based on the efficient thermal ionization of atomic species which have been selectively excited by tunable laser radiation. The performance of LEI for real sample analysis is presently being evaluated. A successful determination of trace Ni concentrations in heavy oil flash distillate and Standard Reference Material Fuel Oil has been performed. One gram samples were diluted into 100-700 mL volumes of a xylene/n-butanol solvent mixture and aspirated directly into an air-acetylene flame. Stepwise laser excitation of Ni was performed using a Nd:YAG pumped dual-dye laser system. Accurate and reproducible results were obtained.

*600,178*
**PB86-207180** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Microbeam Analysis of Samples of Unusual Shape.**
Final rept.,
D. E. Newbury. 1984, 6p
Pub. in Jnl. de Physique (Supplement), v45 n2 p775-780 1984.

Keywords: *Microanalysis, *Particle shape, Electron probes, Correction, Reprints, *Electron microprobe analysis.

Electron probe microanalysis of samples of unusual shape, e.g., particles and rough surfaces, requires correction for the influence of geometric effects on electron scattering, x-ray absorption, and fluorescence. Normalization of the analysis total to unity puts the calculated concentrations on a reasonable bulk basis, but does not uniformly correct the geometric effects as a function of x-ray energy. Peak-to-background ratios are found to be independent of geometric effects to a first order. Correction of measured intensities by use of the background can significantly improve quantitative analysis.

*600,179*
**PB86-209665** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Visibility of Asbestos Fibers in the Scanning Electron Microscope.**
Final rept.,
J. Small, D. Newbury, and R. Myklebust. 1983, 3p
Pub. in Proceedings of Annual Conference of Microbeam Analysis Society (18th), Phoeniz, AZ., August 6-12, 1983, Microbeam Analysis-1983, p148-150.

Keywords: *Asbestos, Contrast, Visibility, *Chrysotile, *Scanning electron microscopy.

Calculations have been made of the contrast of asbestos fibers in a back-scattered plus secondary electron image produced in the scanning electron microscope. From the calculated contrast, the threshold beam current for visibility and the minimum beam diameter have been determined. For chrysotile asbestos on a low atomic number background, fibers below 200 nm diameter are not visible in a rapid scanned image.

*600,180*
**PB86-227113** PC **A11**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Basic Tables for Chemical Analysis.**
Technical note,
T. J. Bruno, and P. D. N. Svoronos. Apr 86, 233p
NBS/TN-1096
Also available from Supt. of Docs as SN003-003-02724-3. Prepared in cooperation with Queensborough Community Coll., Bayside, NY., and Georgetown Univ., Washington, DC. Dept. of Chemistry. Sponsored by Gas Research Inst., Chicago, IL., and Department

of Energy, Washington, DC. Office of Basic Energy Sciences.

Keywords: *Chemical analysis, Tables(Data), Gas chromatography, Infrared spectroscopy, Ultraviolet spectroscopy, Mass spectroscopy, Nuclear magnetic resonance, Qualitative analysis, Liquid column chromatography.

Tables of important data for use in the analytical chemistry laboratory are provided. These tables contain information for use in gas chromatography, liquid chromatography, infrared and ultraviolet spectrophotometry, mass spectrometry, and wet chemical techniques. Tables relating to safe practice in the analytical laboratory are also included.

*600,181*
**PB86-229978** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Comprehensive Method for Determination of Aquatic Butyltin and Butylmethyltin Species at Ultratrace Levels Using Simultaneous Hydridization/ Extraction with Gas Chromatography-Flame Photometric Detection.**
Final rept.,
C. L. Matthias, J. Bellama, G. J. Olson, and F. E. Brinckman. Jun 86, 7p
See also PB86-159555. Sponsored by Office of Naval Research, Arlington, VA., and David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.
Pub. in Environmental Science and Technology 20, n6 p609-615 Jun 86.

Keywords: *Chromatographic analysis, Chemical analysis, Organometallic compounds, Biocides, Water pollution, Chesapeake Bay, Tin organic compounds, Reprints, *Tin/butyl, *Tin/butyl-methyl.

An ultratrace method for the analysis of aquatic anthropogenic butyltin and mixed methylbutyltin species using simultaneous hydridization with sodium borohydride and extraction into dichloromethane is described. The detection limits for a 100-mL sample are 7 ng of Sn/L for tetrabutyltin, 7 ng of Sn/L for tributyltin, 3 ng of Sn/L for dibutyltin, and 22 ng of Sn/L for monobutyltin. Detection limits of approximately 1-2 ng of Sn/L for tri- and tetrabutyltin and less than 1 ng of Sn/L for dibutyltin species were achieved with 800-mL samples. The presence of tetrabutyltin in harbor waters is reported.

*600,182*
**PB86-230505** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Investigations of Selectivity in RPLC (Reversed-Phase Liquid Chromatography) of Polycyclic Aromatic Hydrocarbons.**
Final rept.,
L. C. Sander, and S. A. Wise. 1986, 80p
Pub. in Advances in Chromatography 25, p139-218 1986.

Keywords: *Chromatographic analysis, *Aromatic polycyclic hydrocarbons, Selectivity, Reprints, Reverse phase chromatography, Liquid chromatography.

Selectivity in reversed-phase liquid chromatography (LC) of polycyclic aromatic hydrocarbons (PAH) is affected by both stationary phase parameters (phase type, pore size, and C18 surface coverage) and solute parameters (shape and non-planarity). Polymeric C(18) phases have been shown to have greater selectivity for the separation of PAH than the more commonly used monomeric C(18) phases. In the chapter, the recent investigations of reversed-phase LC selectivity for PAH will be reviewed and discussed including: bonded phase syntheses, characterization of substrate and bonded phase properties, and the effect of such parameters on selectivity.

*600,183*
**PB86-231560** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Software for Data Collection and Analysis from a Size-Exclusion Liquid Chromatograph.**
Final rept.,
J. D. Barnes, B. Dickens, and F. L. McCrackin. 1985, 10p
Pub. in Computer Applications in the Polymer Laboratory, Chapter 13, p130-139 1985.

Keywords: Molecular weight, Surveys, Exclusion, Fortran, Automation, *Liquid chromatography, Computer software, Separation processes, Computer applications.

The paper describes software that is used for data collection and analysis from size-exclusion liquid chromatograph. The chromatograph is a commercially available instrument that provides on board microprocessor control of the specimen injection functions. They use a commercially available microcomputer as a passive listener connected to the chromatograph output to collect, store, and analyze the data. The data collection and analysis software is written in FORTRAN. Maximum use is made of graphical displays to aid the user's judgement in interpreting the data. All operations are menu drive, so that the user does not need to be familiar with the computer's operating system. Data archiving functions are built in to facilitate after-the-fact retrieval of the data.

*600,184*
**PB86-239126** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Quality Assurance Techniques for Activation Analysis.**
Final rept.,
D. A. Becker. 1984, 10p
Pub. in Proceedings of Int. Conf. Nucl. Methods Environ. Energy Res. (5th), p657-666 1984.

Keywords: *Neutron activation analysis, Chemical analysis, Quality assurance, Standards, Data processing, Calibration.

The principles and techniques of quality assurance are applied to the measurement method of activation analysis. Quality assurance is defined to include quality control and quality assessment. Plans for quality assurance include consideration of: personnel; facilities; analytical design; sampling and sample preparation; the measurement process; standards; and documentation. Activation analysis concerns include: irradiation; chemical separation; counting/detection; data collection and analysis; and calibration. Types of standards discussed include calibration materials and quality assessment materials.

*600,185*
**PB86-239373** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Vortex Cooling for Subambient Temperature Gas Chromatography.**
Final rept.,
T. J. Bruno. 1986, 1p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in Analytical Chemistry 58, p1596 1986.

Keywords: *Gas chromatography, *Hilsch tube, Reprints, *Vortices.

There has been a good deal of recent interest in subambient temperature gas chromatography, especially for work involving priority pollutants present in air samples. The most popular method of achieving subambient temperatures in chromatographic ovens is through the use of a cryogenic fluid. The short note describes the use of the Ranque-Hilsch vortex tube as a simple and effective alternative to liquefied gases when column temperatures of between -40 and 0 deg C are required.

*600,186*
**PB86-247632** PC **A03**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Computer Software for the Acquisition and Treatment of Calorimetric Data.**
Technical note (Final),
D. K. Steckler, R. N. Goldberg, Y. B. Tewari, and T. J. Buckley. May 86, 45p NBS/TN-1224
Also available from Supt. of Docs as SN003-003-02748-1.

Keywords: *Calorimeters, *Heat measurement, Data acquisition, Data processing, Thermodynamic properties, Measuring instruments, Chemical analysis, *Computer software, Computer program documentation, Calorimetry.

The computer software used for the acquisition and treatment of data from both heat-conduction microcalorimeters and an isoperibol solution calorimeter is described. For each program contained there is documentation given which includes a listing of the program, comments, and an example of its use. The hardware used in the data acquisition is briefly described.

*600,187*
**PB87-100194**
(Order as PB87-100186, PC **A08**/MF **A01**)
National Bureau of Standards, Boulder, CO.
**High Precision Microcalorimetry: Apparatus, Procedures, and Biochemical Applications,**
D. K. Steckler, R. N. Goldberg, Y. B. Tewari, and T. J. Buckley. 25 Feb 86, 9p
Included in Jnl. of Research of the National Bureau of Standards, v91 n3 p113-121 May-Jun 86.

Keywords: *Chemical analysis, *Heat measurement, Biochemical reaction kinetics, Thermal measuring instruments, Chemical reactions, Enzymes, *Calorimetry.

Apparatus and procedures used for high-precision microcalorimeter is of the heat-conduction type and utilizes semi-conductor thermoelectric modules. The biocompartmental reaction vessel is made of high-density polyethylene and holds about 0.5 mL of solution in each compartment. Imprecision of heat measurement is 0.2 percent when measuring 300 mJ of heat produced by a rapid chemical reaction. Three microcalorimeters are operated simultaneously using a microcomputer and a data acquisition system. Theromchemical and kinetic applications are described. The acquisition of data from an isoperibol solution calorimeter is also described.

*600,188*
**PB87-100202**
(Order as PB87-100186, PC **A08**/MF **A01**)
National Bureau of Standards (NEL), Boulder, CO.
**Standards Development for Differential Scanning Calorimetry,**
J. E. Callanan, S. A. Sullivan, and D. F. Vecchia. Jun 86, 7p
Included in Jnl. of Research of the National Bureau of Standards, v91 n3 p123-129 May-Jun 86.

Keywords: *Heat measurement, *Thermal analysis, Enthalpy, Standards, Transition temperature, Calibration, Differential scanning calorimetry.

The article summarizes two studies made in preparation for standards development, by differential scanning calorimetry, for instruments such as scanning calorimeters, differential thermal analyzers, differential mechanical analyzers, and related thermal analysis devices. The first was an extensive study of the varability of differential scanning calorimeters when used for determining transition temperatures and enthalpies. The second was an evaluation of calibration procedures recommended by the American Society of Testing and Materials. These studies are described in detail in National Bureau of Standards Special Publication 260-99.

*600,189*
**PB87-104261** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Miniature Mercury Contact Switch for Chromatographic Applications.**
Final rept.,
T. J. Bruno, and J. G. Shepherd. Mar 86, 1p
Sponsored by Gas Research Inst., Chicago, IL., and Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Analytical Chemistry 58, n3, p672 Mar 86.

Keywords: *Chemical analysis, *Temperature control, *Gas chromatography, *Electric switches, Mercury, Reprints.

A small mercury contact switch for use in temperature control of gas chromatographic equipment has been designed and constructed. The major features of the device are described, including its present limitations. The results of preliminary testing of the device are also given.

*600,190*
**PB87-105813** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.

**Chemometrics and Analytical Chemistry.**
Final rept.,
L. A. Currie. 1984, 32p
Pub. in NATO ASI Ser., Ser. C, Chemometrics 138, p115-146 1984.

Keywords: *Chemical analysis, Quality control, Measurement, Reprints, *Chemometrics.

Modern analytical chemistry has become intrinsically tied to the exposure, understanding, and resolution of many of today's sociotechnical problems, in areas ranging from medical diagnostics to guarding our climate. Chemometrics is central in deriving adequate responses to these needs in terms of the design, control, evaluation and validation of the analytical measurement process. In the two reprints which follow, the substance of the lecture is treated in the first (I) while the second (II) comprises a case study from the relatively new discipline of 'Chemometric Intercomparison', or interlaboratory (numerical) validation via simulated analytical data. The paragraphs which follow are offered to introduce the reprints and to summarize some recent observations on the subject of detection.

*600,191*
**PB87-106118** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Appilcation of Capillary Gas Chromatography-Mass Spectrometry to Chemical Characterization of Radiation-Induced Base Damage of DNA: Implications for Assessing DNA Repair Processes.**
Final rept.,
M. Dizdaroglu. 1985, 11p
Pub. in Analytical Biochemistry 144, n2 p593-603 1985.

Keywords: *Chromatographic analysis, *Deoxyribonucleic acids, Gas chromatography, Mass spectroscopy, Reprints, *Radiation effects, DNA damage, Biological repair.

The application of capillary gas chromatography-mass spectrometry (GC-MS) to the chemical characterization of radiation-induced base products of calf thymus DNA is presented. Samples of calf thymus DNA irradiated in N2O- saturated aqueous solution were hydrolyzed with HCOOH, trimethylsilylated and subjected to GC-MS analysis using fused silica capillary column. The trimethylsilyl derivatives of these products had excellent GC-properties and easily interpretable mass spectra, where an intense molecular ion M(1+) and a charateristic (M-CH3) ion were observed. Using the methodology, it was possible to show the formation of novel base products in irradiated DNA in addition to the products reported previously. All mass spectra obtained were discussed in detail. The capillary GS-MS using the methodology described here was suggested as a very suitable technique for investigation of DNA repairability by repair mechanisms of DNA lesions created by either ionizing radiation or other agents, e.g., chemical mutagens, oxidizing agents, etc.

*600,192*
**PB87-106423** PC **A04**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Collection of Abstracts of Selected Publications Related to Quality Assurance of Chemical Measurements,**
J. K. Taylor. Apr 86, 52p NBSIR-86/3352

Keywords: *Chemical analysis, *Quality assurance, Quality control, Accuracy, Precision, Reference materials.

The publication contains abstracts of 150 papers selected for their usefulness to analytical chemists, laboratory managers, and quality assurance officials when developing new or improving existing programs or for general guidance in producing reliable analytical chemical measurements. Definitions of some 75 terms used in describing the quality aspects of chemical measurements are included.

*600,193*
**PB87-106704** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
**Certified Reference Materials for Validating Spectroscopic Methods and Experimental Data.**
Final rept.,
R. Alvarez. 1986, 8p
Pub. in Fresenius Zeitschrift fuer Analytische Chemie 324, p376-383 1986.

Keywords: *Spectroscopic analysis, Chemical analysis, Calibrating, Standards, Reprints, *Standard reference materials, Certified reference materials.

Chemical analyses of the same homogeneous materials by different laboratories often disagree. Discrepant data may be caused by poor methodology, improper instrument calibration, faulty experimental techniques, impure reagents, or from a combination of these factors. For trace constituent determinations, the magnitude and evaluation of the method blank are often the main limitations toward obtaining accurate results. One approach towards improving the accuracy of analytical determinations is by the use of Certified Reference Materials (CRMs) issued by organizations throughout the world. A CRM is a homogeneous, stable material with certified chemical and/or physical properties used in calibrating instruments, validating experimental data, developing methods of known reliability, and referring data from different laboratories to a common base. In the United States, the National Bureau of Standards has legal authority to issue CRMs, which for historical reasons are called Standard Reference Materials (SRMs).

*600,194*
**PB87-107157** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Vortex Refrigeration of HPLC (High Performance Liquid Chromatography) Components.**
Final rept.,
T. J. Bruno. 1985, 2p
Sponsored by Department of Energy, Washington, DC.
Pub. in Liquid Chromatography 4, n2 p134-136 1985.

Keywords: *Chromatographic analysis, *Hilsch tubes, Cooling, Reprints, High pressure liquid chromatography.

Due to the recent interest in cooling the components of HPLC and SFC instrumentation, an approach to component cooling based on vortex refrigeration is presented. The refrigeration units described use the Ranque-Hilsh vortex tube to generate cold air with which to cool chromatographic components. A discussion of the operation of the refrigeration units is provided, and the problem of noise is addressed.

*600,195*
**PB87-107298** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Two-Dimensional Proton Chemical Shift Correlated NMR Spectroscopy of Digitoxose.**
Final rept.,
B. Coxon. 1984, 19p
Pub. in J. Carbohydr. Chem. 3, n4 p525-543 1984.

Keywords: *Spectroscopic analysis, Chemical analysis, Nuclear magnetic resonance, Carbohydrates, Reprints, *Chemical shift, *Digitoxose, Two dimensional.

The hydroxyl proton coupled 1H NMR spectra of solutions of beta-D-digitoxopyranose and of an equilibrated mixture of the four ring forms of D-digitoxose in dimethyl-sulfoxide-d sub 6 have been assigned completely by two-dimensional, proton chemical shift correlated NMR spectroscopy and spin decoupling at 400 MHz. Analysis of resolution enhanced, one-dimensional (1)H NMR spectra yielded an almost complete set of CH and OH proton-proton coupling constants for the four ring forms. The free aldehydo form of D-digitoxose in dimethylsulfoxide-d sub 6 solution has been detected by means of its characteristic H-1 quartet at 9.687. Quantitative analysis of the equilibrated mixture of the five forms of D-digitoxose gave the composition: - alpha-pyranose, beta-pyranose, alpha-furanose, beta-furanose, aldehydo form, 11.2, 67.3, 8.4, 13.0, and 0.13 percent, respectively.

*600,196*
**PB87-107306** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Two-Dimensional Proton J-Resolved NMR Spectroscopy of Neomycin B.**
Final rept.,
R. E. Botto, and B. Coxon. 1984, 19p
Pub. in J. Carbohydro. Chem. 3, n4 p545-563 1984.

Keywords: *Spectroscopic analysis, Chemical analysis, Nuclear magnetic resonance, Antibiotics, Reprints, *Chemical shift, *Neomycin B, Coupling constants, Two dimensional.

The (1)H NMR spectrum of a solution of neomycin B free base (Structure 1) in D2O has been assigned completely by two-dimensional, homonuclear J-resolved NMR spectroscopy and spin decoupling at 400 MHz. Proton chemical shifts and proton-proton couplings are reported for all glycoside residues in neomycin B along with their computer simulated spectra. The (4)C1, chair conformation has been assigned to the pyranose form of the 2,6-diamino-2,6-dideoxy-alpha L-idosyl (ring D) portion of the antibiotic (1b) by analysis of the proton coupling constants and chemical shifts. The beta-furanose form of the ribosyl portion (ring C) has been assigned. Vicinal proton couplings for the 2-deoxystreptaminyl group (ring B) are consistent with a chair conformation in which all ring substituents are equatorial, and proton chemical shift assignments are based on protonation studies. A computer simulated composite of the individual calculated spectra is presented for comparison with the experimental spectrum of neomycin B.

*600,197*
**PB87-107322** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Nonlinear Effects of Digitizer Errors in FT-IR (Fourier Transform Infrared) Spectroscopy.**
Final rept.,
A. Baghdadi, W. K. Gladden, and D. R. Flach. 1986, 12p
Pub. in Applied Spectroscopy 40, n5 p617-628 1986.

Keywords: *Infrared spectrometers, *Spectroscopic analysis, *Analog to digital converters, Chemical analysis, Infrared spectroscopy, Accuracy, Errors, Reprints, Fourier transform spectroscopy, Nonlinear problems.

The paper is an investigation of the effects of errors in the analog-to-digital converter (ADC) of a Fourier transform infrared (FT-IR) spectrometer on the photometric accuracy of that spectrometer. The effect of ADC errors on the spectrum after Fourier transformation is calculated analytically for monochromatic, two-line, and wide square band emission spectra. Numerical modeling is used to extend the analysis to absorption spectra, and to include the effects of noise on the amplitude of absorbance bands. These analyses showed that ADC errors can generate artifacts throughout the spectrum, although the largest effects occur at sharp spectral features.

*600,198*
**PB87-109492** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Mass Spectrometry of 2-Methylthio(Glyco)Oxazoline Derivatives of Pentoses and Hexoses.**
Final rept.,
G. D. Byrd, R. M. Davidson, E. White, V. B. Coxon, and S. A. Margolis. 1985, 5p
Pub. in Organic Mass Spectrometry 20, n7 p458-462 1985.

Keywords: *Chemical analysis, *Pentoses, *Hexoses, Mass spectroscopy, Carbohydrates, Metastable state, Reprints, *Oxazoline/(glyco)-methylthio.

The fragmentation of 2-methylthio(glyco)oxazolines under electron impact has been investigated by low and high resolution mass spectrometry. Field desorption was used in those cases where the molecular ion was weak or missing. Fragmentation pathways were determined by monitoring metastable transitions and through the use of labeled compounds. The results support the anticipated structure for these compounds and show the sensitivity of the mass spectra toward ring size.

*600,199*
**PB87-109526** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Impact of Instrumentation on Analytical Chemistry.**
Final rept.,
J. K. Taylor. 1986, 10p
Pub. in the History and Preservation of Chemical Instrumentation, p1-10 1986.

Keywords: *Chemical analysis, Quality assurance.

The analytical chemist has always depended on instrumentation and has been limited by instrumental capa-

bility. Advances in instrumentation during recent times have led to new capabilities in trace analysis, high accuracy analysis, multicomponent analysis, and analytical process control that could hardly have been imagined only a few years ago. The impact on the analyst has resulted in his transition from a generalist to a specialist and the production of data from an individual to a sub-contractor mode of operation. The result has been the need for formalized quality assurance practices if data are to be compatible. Only in the most routine situations is the need for competent analysis decreasing. Rather, the complexity of modern analysis is requiring a higher-than-ever level of competence of analysts practicing at the highest levels of professionalism.

*600,200*
**PB87-109534** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Validation of Analytical Data.**
Final rept.,
J. K. Taylor. 1986, 5p
Pub. in Marine Chemistry 18, p115-119 1986.

Keywords: *Chemical analysis, Proving, Marine atmospheres, Quality assurance, Environmental surveys, Reprints.

Valid data may be defined as those which result from a valid measurement process applied to valid samples, selected in accordance with a valid plan based on a valid model of the problem under investigation. The paper discusses the various aspects of the validation process.

*600,201*
**PB87-109542** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Guidelines for Evaluating the Blank Correction.**
Final rept.,
J. K. Taylor. Jan 84, 2p
Pub. in Jnl. of Testing and Evaluation 12, n1 p54-55 Jan 84.

Keywords: *Chemical analysis, *Trace elements, Guidelines, Water, Reprints.

The statistical considerations in applying the blank correction in trace analysis are discussed. The question of acceptable limits for the blank is addressed. Unless sufficient measurements are made, the uncertainties in the blank correction may be the major source of uncertainty in ultra-trace analysis.

*600,202*
**PB87-110169** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Techniques for the Calibration of Microscopic Particle Size Standards.**
Final rept.,
D. A. Swyt, T. R. Lettieri, A. W. Hartman, and S. W. Jensen. 1983, 12p
Pub. in Particulate Systems, p335-346 1983.

Keywords: *Particle size distribution, *Standards, *Chemical analysis, Calibration, Electron microscopy, Particle size, Reprints.

Three methods for the measurement of size distributions of microscopic spherical particles - light scattering, electron microscopy, and flow counting - form a complementary set of techniques under development for use at the National Bureau of Standards for calibration of polymer spheres as particle size standards.

*600,203*
**PB87-111829** PC **A08**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Proceedings of the 1986 Meeting of the Americas Branch of the Electrophoresis Society, March 16-28, 1986,**
D. J. Reeder. Mar 86, 172p NBSIR-86/3345

Keywords: *Meetings, *Chemical analysis, Peptides, Nucleic acids, Molecular weight, Staining, *Electrophoresis, Isoelectric focusing, Immobilized pH gradients.

The publication consists of submitted plenary papers and abstracts for the 1986 Meeting of the Americas Branch of the Electrophoresis Society. The plenary papers are in-depth reviews and comprise 80% of the document.

*600,204*
**PB87-117701** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Application of Neutron Depth Profiling to Microelectronic Materials Processing.**
Final rept.,
R. G. Downing, J. T. Maki, and R. F. Fleming. 1986, 18p
Pub. in American Chemical Society Symposium Series 295, p163-180 1986.

Keywords: *Chemical analysis, Depth finding, Helium, Lithium, Beryllium, Boron, Sodium, Bismuth, Microelectronics, *Neutron depth profiling.

Thermal neutron depth profiling (NDP) provides an isotope specific, nondestructive technique for the measurement of concentration versus depth distributions in the near-surface region of solids. The profiles are generated in real-time, analyzing depths of up to tens of micrometers. The method is particularly sensitive for the investigation of He, Li, Be, B, Na and Bi profiles. Demonstrative applications are presented for the technique, including: ion implantation-anneal sequence profiling; diffusion studies in a number of microelectronic materials; and homogeneity analysis of thin glass film overcoats. Comparisons are made for NDP and other profiling techniques such as secondary ion mass spectrometry (SIMS), Rutherford backscattering (RBS) and spreading resistance profiling (SRP).

*600,205*
**PB87-118568** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Determination of Pore Accessibility in Silica Microparticles by Small Angle Neutron Scattering.**
Final rept.,
C. J. Glinka, L. C. Sander, S. A. Wise, M. L. Hunnicutt, and C. H. Lochmueller. 1985, 6p
Pub. in Analytical Chemistry 57, n11 p2079-2084 1985.

Keywords: *Porosity, *Silica gel, *Chemical analysis, Neutron scattering, Absorbers(Materials), Silicon dioxide, Area, Reprints.

The size, surface area and, in particular, the accessibility of pores in silica particles used in liquid chromatography have been studied by small angle neutron scattering (SANS). From SANS measurements on dry silica samples, values from the specific surface area are obtained and have been compared with BET measurements. Pore accessibility has been studied by saturating the samples with an H2O/D2O solution whose neutron scattering length density matches that of silica. Any residual scattering observed under this condition can be attributed to closed (unfilled) pores. Results are reported for silica particles with nominal pore size ranging from 5 to 33 nm. In addition, other applications of SANS related to the use of porous silica in chromatography and catalysis are discussed.

*600,206*
**PB87-118733** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Role of Neutron Activation Analysis in Trace Analysis.**
Final rept.,
H. L. Rook. 1985, 28p
Pub. in Jnl. of Trace and Microprobe Techniques 2, n3-4 p189-216 1984-85.

Keywords: *Neutron activation analysis, *Trace elements, Chemical analysis, Radioactivation analysis, Reprints.

Neutron activation analysis is a technique which has become widely accepted for trace element analysis. It combines the advantages of high sensitivity, minimal matrix dependence and relative simplicity in analytical procedure. The combination of instrumental neutron activation analysis and radiochemical neutron activation analysis now allows the analysis of more than fifty elements in real samples. To illustrate this, the capability of neutron activation is reviewed considering a series of NBS botanical, biological, and geochemical Standard Reference Materials from the perspective of elemental sensitivity, elemental coverage, and analytical accuracy.

*600,207*
**PB87-122214** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
**Nuclear Methods--An Integral Part of the NBS (National Bureau of Standards) Certification Program.**
Final rept.,
T. E. Gills. 1984, 10p
Pub. in Proceedings of International Conference on Nuclear Methods in Environmental and Energy Research (5th), Mayaguez, Puerto Rico, April 2, 1984, p634-643.

Keywords: Radioactivation analysis, Measurement, Accuracy, *Standard reference materials.

Within the past twenty years, new techniques and methods have emerged in response to new technologies that are based upon the performance of high-purity and well-characterized materials. The National Bureau of Standards, through its Standard Reference Materials (SRM's) Program, provides standards in the form of many of these materials to ensure accuracy and the compatibility of measurements throughout the U.S. and the world. These standards, defined by the National Bureau of Standards as Standard Reference Materials (SRM's), are developed by using state-of-the-art methods and procedures for both preparation and analysis. Nuclear methods-activation analysis-constitute an integral part of that analysis process.

*600,208*
**PB87-122818** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**NBS (National Bureau of Standards) Standard Reference Materials for Improving the Accuracy of Priority Pollutant Analyses.**
Final rept.,
B. I. Diamondstone. 1981, 9p
Pub. in Proceedings of Seminar for Analytical Methods for Priority Pollutants, Hershey, PA., April 9-10, 1981, p186-194.

Keywords: *Chemical analysis, Standards, Accuracy, Quality assurance, Precision, Aromatic polycylic hydrocarbons, *Standard reference materials, *Priority pollutants.

The use of Standard Reference Materials or Quality Assurance Standards as part of an overall quality assurance program can contribute significantly to improvements in both precision and accuracy for many studies being carried out in the areas of environmental measurement and management. A considerable number of standards have been produced in which constituents, of interest to analysts in the environmental field, have been fully characterized. A considerable effort at NBS has gone into the determination of both organics and inorganics in a wide variety of matrices. Many of these constituents presently appear on the EPA list of priority pollutants and therefore, are of significant value to analysts involved with measurements in the area of hazardous wastes. Because of the increased need for standards in this field, long term planning is required in order to meet future demands.

*600,209*
**PB87-122859** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**High Accuracy/High Precision Determination of (235)U in Nondestructive Assay Standards by Gamma-Ray Spectrometry.**
Final rept.,
R. R. Greenberg, and B. S. Carpenter. 1984, 13p
Pub. in Proceedings of International Conference on Nuclear Methods in Environmental and Energy Research (5th), Mayaguez, Puerto Rico, April 2, 1984, p644-656.

Keywords: *Chemical analysis, *Uranium 235, Standards, Accuracy, Precision, Reprints, *Standard reference materials, Gamma spectroscopy, Isotope abundance.

High precision gamma spectrometry measurements have been made on five sets of five uranium isotope abundance reference materials for nondestructive assay (NDA). These sets are intended for international safeguards use as primary reference materials for the determination of the (235)U abundance in homogeneous uranium bulk material by gamma spectrometry. The measurements are to determine the counting rate uniformity of the (235)U 185.7 keV gamma as well as the (235)U isotope abundance for each sample. The results of the study indicate that accuracy of (235)U determination via gamma spectrometry, in the range of few hundredths of a percent (2 sigma), is achievable.

The main requirement for achieving this level of accuracy is a set of standards whose (235)U isotope abundance are known to within 0.01% (2 sigma).

*600,210*
**PB87-128310** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Development of Standard Operating Procedures for Differential Scanning Calorimeters.**
Final rept.,
J. E. Callanan, and S. A. Sullivan. Oct 86, 9p
Pub. in Review of Scientific Instruments 57, n10 p2584-2592 Oct 86.

Keywords: *Chemical analysis, Standards, Calibrating, Operations, Data reduction, Reprints, *Differential scanning calorimetry, Procedures.

The paper describes an assessment of the behavior of a differential scanning calorimeter and the development of satisfactory calibration, operation, and data reduction procedures, which depend on performance characteristics of the individual instrument. Factors that contribute to thermal lag are identified; suggestions for evaluating and compensating for it are given.

*600,211*
**PB87-131504** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Analysis of Nitrogen Heterocycles in Shale Oil by a Dual Capillary Column Heart Cutting Technique.**
Final rept.,
F. R. Guenther, S. N. Chesler, and R. M. Parris. 1986, 7p
Pub. in Jnl. of Chromatography 363, p199-205 1986.

Keywords: *Chromatographic analysis, *Shale oil, *Nitrogen heterocyclic compounds, Chemical analysis, Gas chromatography, Reprints.

The analysis of nitrogen heterocycles in a shale oil matrix is described. A dual column gas chromatograph is used for the analysis after a simple sample preparation scheme is used. Details of the apparatus, especially the intercolumn pneumatic microswitch, are given. Quantitation by the standard addition method using internal volume corrections is described. Future direction for further development of the technique is briefly discussed.

*600,212*
**PB87-132080** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Surface Roughness Metrology by Angular Distributions of Scattered Light.**
Final rept.,
D. E. Gilsinn, T. V. Vorburger, E. C. Teague, M. J. McLay, and C. Giauque. 1985, 14p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in SPIE 525, p2-15 1985.

Keywords: *Surface roughness, *Chemical analysis, Surfaces, Mathematical models, Depth, Measurement, Reprints, Angular distribution.

On-line industrial inspection of batch manufactured parts requires fast measurement techniques for surface finish quality. In order to develop the measurement basis for these techniques, a system has been built to determine surface roughness by measuring the angular distributions of scattered light. The system incorporates data gathered from the angular distribution instrument and traditional surface stylus instruments. These data are used both as input and as comparison data in order to test various mathematical models of optical scattering phenomena. The object is to develop a mathematical model that uses the angular distribution of scattered light to deduce surface roughness parameters such as R(sub a) and surface wavelength. The paper describes the results of an experiment in which angular scattered data from surfaces with sinusoidal profiles was used to compute the surface R(sub a) and wavelength. Stylus measurements of these parameters were made separately. A comparative table is given of the computed and measured values. Estimates of uncertainties are also given.

*600,213*
**PB87-132684** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Precise and Accurate Determination of the (241)Pu Half-Life by Mass Spectrometry.**
Final rept.,
W. R. Kelly. 1985, 6p
Pub. in International Jnl. of Mass Spectrometry and Ion Processes 64, n1 p85-90 1985.

Keywords: *Chemical analysis, *Mass spectroscopy, *Half life, Precision, Accuracy, Reprints, *Plutonium 241, Americium 241.

A mass spectrometric procedure is proposed and described which eliminates biases due to the isobaric interference of (241) Am and mass dependent fractionation effects in the determination of the (241) Pu halflife. An equal atom mixture of Pu isotopes is prepared and aliquots are spiked with high purity (243) Am after a Pu-Am chemical separation. The (241)AM(1+) contribution to the (241)Pu(1+) ion current is determined by measuring the (243)Am(1+) ion current. The (244)Pu/(239)Pu ratio is used as an internal standard to correct the measured (241)Pu/(sup i)Pu ratios for mass fractionation. The use of these procedures will result in a determination that is under complete statistical control and will yield a highly accurate and precise value. It is estimated that the uncertainty using these techniques would be about 0.001 years (1 sigma(sub m) after a decay interval of only 3 years.

*600,214*
**PB87-132692** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Supercritical Fluid Extraction Procedure for the Removal of Trace Organic Species from Solid Samples.**
Final rept.,
M. M. Schantz, and S. N. Chesler. 1986, 5p
Pub. in Jnl. of Chromatography 363, p397-401 1986.

Keywords: *Chromatographic analysis, *Aromatic polycyclic hydrocarbons, Chemical analysis, Gas chromatography, Extraction, Reprints, *Polychlorinated biphenyls, NBS sediments.

The supercritical extraction of polychlorinated biphenyls (PCBs) from sediments and poly aromatic hydrocarbons (PAHs) from an urban particulate sample (NBS SRM 1649) is described. A commercial supercritical fluid chromatograph, designed for use with packed columns, is employed for temperature and pressure control, and a gas chromatograph equipped with either an electron capture detector or flame ionization detector is used for the PCB or PAH analysis, respectively. The supercritical extraction is compared to Soxhlet extraction for the sediment material and to certified values for the urban dust.

*600,215*
**PB87-132700** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Identification and Quantitation of the Impurities in Sodium Pyruvate.**
Final rept.,
S. A. Margolis, and B. Coxon. 1986, 7p
Pub. in Analytical Chemistry 58, n12 p2504-2510 Oct 86.

Keywords: *Chemical analysis, Impurities, Nuclear magnetic resonance, Reprints, *Pyruvic acid/(Sodium-salt), Carbon 13.

Sodium pyruvate has been resolved from its acyclic dimer and oligomers by chromatography on Sephadex G-15. The compositions of the monomer, the dimer, and the synthetic dimer have been characterized by means of their carbon-13 and proton NMR spectra. The ultraviolet spectra and the absorptivities were also measured. By use of the molar absorptivities, the levels of the acyclic dimer have been calculated from the chromatograms of several commercial preparations of sodium pyruvate. The purest sodium pyruvate sample was selected for certification as NBS Standard Reference Material 910, for use as a substrate for the assay of enzymes of clinical importance.

*600,216*
**PB87-132726** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Precise and Accurate Determination of High Concentrations of Sulfur by Isotope Dilution Thermal Ionization Mass Spectrometry.**
Final rept.,
W. R. Kelly, and P. J. Paulsen. 1984, 6p
Pub. in Talanta 31, n12 p1063-1068 1984.

Keywords: *Sulfur, *Chemical analysis, Steels, Reprints, Isotope dilution.

An isotope dilution thermal ionization mass spectrometric procedure has been developed for the accurate and precise determination of S in steels and organic based materials. Samples are dissolved in a sealed tube to prevent loss of S and the S isotopes are measured as the As S (1+) molecular ion, using silica gel as an emitter. The technique has been applied to the determination of S in 13 SRM's. The total uncertainty is typically 0.5% (95% confidence interval) and is governed by the uncertainty in the spike calibration and sample homogeneity.

*600,217*
**PB87-134771** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Characterization of Airborne Particulates by Pyrolysis/Mass Spectrometry and Carbon-14 Analysis.**
Final rept.,
K. J. Voorhees, S. M. Kunen, S. L. Durfee, L. A. Currie, and G. A. Klouda. 1981, 3p
Pub. in Analytical Chemistry 53, n9 p1463-1465 1981.

Keywords: *Chemical analysis, Carbon 14, Pyrolysis, Mass spectroscopy, Oil shale, Aerosols, Reprints, *Particulate sampling, Radiocarbon, Oil shale dusts.

Pyrolysis/mass spectromety (Py/MS) has been used to characterize the composition of organics in an ambient air particulate sample from the eastern Utah oil shale lands. The procedure involved collection of the individual contributors, pyrolysis of these samples, and finally a least-squares fitting of the individual contributor spectra to the pyrolysis mass spectrum of the ambient sample. The Py/MS results were verified by using (14) C analysis.

*600,218*
**PB87-134789** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Accelerator Mass Spectrometry Sample Preparation: Methods for (14)C in 50-1000 Microgram Samples.**
Final rept.,
G. A. Klouda, L. A. Currie, D. J. Donahue, A. J. T. Jull, and T. H. Zabel. 1984, 7p
Pub. in Nuclear Instruments and Methods in Physics Research Section B-Beam Interactions WI 233, n2 p265-271 1984.

Keywords: *Chemical analysis, *Carbon 14, Concentration(Composition), Accuracy, Radioactive isotopes, Mass spectroscopy, Reprints, *Radiocarbon, Iron carbon alloy.

A joint project was undertaken by the National Bureau of Standards (NBS) Atmospheric Chemistry Group and University of Arizona (UoA) Tandem Accelerator Mass Spectrometer Group to develop and evaluate accelerator (14)C measurements of 50 to 1000 microgram carbon samples at a modest accuracy of 5 to 10% Fe-C alloy targets prepared from standards and samples averaged 1.6 microamps (12)C-current. (14)C measurements yielded 10% precision and accuracy, limited by a blank equivalent to 11% modern carbon for targets containing -100 mi carbon. The contamination level was estimated to be -15 mi contemporary carbon (current atmospheric (14)C). The results demonstrated that the Fe-C target is quite suitable for atmospheric and environmental studies that require measuring fossil/biogenic carbon in microgram samples.

*600,219*
**PB87-134797** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
**Standard Reference Materials (SRM) In Chemical Monitoring Systems.**
Final rept.,
W. P. Reed, and T. E. Gills. 1986, 4p
Pub. in Proceedings of OCEANS 86 Monitoring Strategies Symposium, Washington, DC., September 23-25, 1986, v3 p814-817.

Keywords: *Chemical analysis, Standards, Monitors, Oceanography, *Standard reference materials.

The need for standards for physical measurements has been recognized as far back as the days of the Egyptian pharaohs and the use of the cubit as a unit of length. Since that time, increased measurement so-

phistication has led to the need for accurate physical standards of measurement. The development of the metric system and subsequently the International System of Units (SI), has in many ways met the need for primary standards for physical measurements. The accurate measurement of chemical properties is a more recent need. The paper explores the use of chemical measurement systems and their role in obtaining and verifying highly accurate and precise measurements over a long period of time. Also included in the discussion is a review of currently available Standard Reference Materials appropriate to ocean science and monitoring.

*600,220*
**PB87-137162**
(Order as PB87-137154, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Temperature Dependence of Spectral Broadening in the Hg (6 singlet S(sub 0) - 6 triplet P(sub 1) Multiplet at High Optical Densities,**
W. Braun, M. D. Scheer, and V. Kaufman. 10 Jul 86, 9p
Included in Jnl. of Research of the National Bureau of Standards, v91 n6 p313-321 Nov-Dec 86.

Keywords: *Mercury(Metals), *Chemical analysis, Absorption, Calibration, Gases, *Temperature dependence.

A new method has been developed for determining rapidly changing translational temperatures in a gas that has been heated by such transient phenomenena as the passage of shock wave or the absorption of sub-microsecond pulses of radiation from an infrared laser. The method depends upon the use of trace amounts of Hg vapor and its absorption of radiation in the neighborhood of the 253.7 nm isotopic and hyperfine multiplet. As the Hg atoms sense changes in the translational temperature of the host gas, the absorption of 253.7 nm radiation also changes by virtue of the Doppler and Lorentz broadening of the multiplet lines. Emission spectra of a Hg discharge light source in the neighborhood of 253.7 nm were shown to be readily simulated by a two zone computer model even at large optical densities. This provided a means for obtaining the temperature calibration curves needed to monitor the changing translational temperature of a gas undergoing rapid heating or cooling.

*600,221*
**PB87-140224** PC **A06**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Technical Activities 1986, Molecular Spectroscopy Division,**
A. Weber. Nov 86, 108p NBSIR-86/3483
See also PB86-164381.

Keywords: *Molecular spectroscopy, Resolution, Chemical analysis, Research projects, Frequency standards, Quantum chemistry, Photochemical reactions.

The report summarizes the technical activities of the NBS Molecular Spectroscopy Division during the Fiscal Year 1986. The activities span experimental and theoretical research in high resolution molecular spectroscopy, quantum chemistry and laser photochemistry, and include the development of frequency standards, critically evaluated spectral data, applications of spectroscopy to important scientific and technological problems, and the advancement of spectroscopic measurement methods and techniques. A listing is given of publications and talks by the Division staff.

## Basic & Synthetic Chemistry

*600,222*
**PB86-186756** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Alkenoxy Radicals in Gas-Phase Reactions of Alkenes with Oxygen Atoms or Ozone.**
Final rept.,
R. I. Martinez. 1983, 4p
Pub. in Jnl. of Chemical Physics Letters 98, n5 p507-510 1983.

Keywords: *Alkene compounds, *Ozone, Chemical radicals, Reaction kinetics, Reprints, *Oxygen atoms, *Free radicals, Chemical reaction mechanisms.

Observations in the O3-trans-2-butene reaction system and in the O+trans-2-butene+O2 reaction system suggest the intermediacy of alkenoxy radicals. A mechanism is proposed for the production of Cn and Cm(m<n) alkenoxy radicals by the reaction of CnH2n alkenes with oxygen atoms or with ozone.

*600,223*
**PB86-189875** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**International Butyltin Measurement Methods Intercomparison: Sample Preparation and Results of Analyses,**
W. R. Blair, G. J. Olson, and F. E. Brinckman. Feb 86, 58p NBSIR-86-3321
Sponsored by Office of Naval Research, Arlington, VA.

Keywords: *Tin organic compounds, Chemical analysis, Environmental impact assessments, Quantitative analysis, Water pollution, Molecular structure, *Stannane/tributyl.

A comparison of prevalent organotin measurement methods has been conducted on an international scale with a new tri-n-butyltin research material distributed to over 40 participating laboratories worldwide. A description of background research into the behavior and manipulation of low-concentration (ppm) aqueous organotin solutions, chromatographic production and packaging of the stable speciated butyltin research material in water, and quantitative results from the international methods intercomparison are reported here along with recommendations for future work.

*600,224*
**PB86-190626** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Coordination Compounds of Benzotriazole and Related Ligands.**
Final rept.,
J. Reedijk, A. R. Siedle, R. A. Velapoldi, and J. A. M. VanHest. 1983, 10p
Pub. in Inorganica Chimica Acta 74, p109-118 1983.

Keywords: *Coordination compounds, *Ligands, *Corrosion prevention, Complex compounds, Transition metals, Reprints, *Benzotriazoles.

The coordination chemistry of benzotriazole towards several transition-metal compounds has been studied. Upon reaction of neutral benzotriazole (BTAH) with metal compounds under varying conditions, both neutral (BTAH) ligands and anionic, depronated ligands (BTA)(1-) may be coordinated to the metal. The compounds have the general formula M(BTAH)(sub n)(X sub m), with M = Cu,Zn,Cd,Hg,Pd,Ti,Sn,n=1, 2,3,4,X = Cl,Br and m = 2 or 4. Similar compounds of formula Cu(ligand)(sub n)(X sub ), (X = Cl,Br; n = 1,2) with 5-nitrobenzotriazole and N-methylbenzotriazole, were obtained. Structures of the compounds have been proposed based on infrared and far-infrared spectroscopy, ligand-field and UV spectroscopy, EPR spectroscopy, conductivity data and NMR-spectroscopy. The bonding modes for the mono-, bi-, and tridentate species are discussed. Polymeric structures using BTA and BTAH as bridging ligands are discussed in relation to the corrosion-inhibiting properties of benzotriazole.

*600,225*
**PB86-192168** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Fourier Transform Infrared Study of the Gas-Phase Reactions of (18)O3 with Trans-CHCl=CHCl In (16)O2-Rich Mixtures. Branching Ratio for O-Atom Production via Dissociation of the Primary Criegee Intermediate.**
Final rept.,
H. Niki, P. D. Maker, C. M. Savage, L. P. Breitenbach, and R. I. Martinez. 1984, 4p
Pub. in Jnl. of Physical Chemistry 88, n4 p766-769 1984.

Keywords: Chemical reactions, Infrared spectroscopy, Reprints, *Criegee intermediate, *Oxygen atoms, Unimolecular reactions, Fourier transform spectroscopy, Oxygen 18.

Using the FTIR spectroscopic method, the authors identified (16)O3 among the products formed in the gas-phase reaction of (18)O3 with trans-CHCl=CHCl in (16)O2-rich mixtures. The primary yield of (16)O3 was determined to be (17 + or - 3)% of the reactants consumed in the presence of a Cl-atom scavenger such as C2H6 or n-C4H10. The finding can be explained by the formation of atomic oxygen in the unimolecular dissociation of the Criegee intermediate H(Cl)COO, i.e., (18)O3 + trans-CHCl=CHCl -> H(Cl)C(18)O(18)O + H(Cl)C=(18)O (1); H(Cl)C(18)O(18)O -> (18)O(3P) + H(Cl)C=(18)O (2); (18)O (2); (18)O + (16)O2 -> (16)O + (16)O9180O (5); and (16)O + (16)O2 (+M) -> (16)O3 (+M) (3).

*600,226*
**PB86-192531** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Calculated Proton Affinities for Some Molecules Containing Group VIA Atoms.**
Final rept.,
P. G. Jasien, and W. J. Stevens. 1985, 6p
Pub. in Jnl. of Chemical Physics 83, n6 p2984-2989, 15 Sep 85.

Keywords: Molecules, Sulfur, Selenium, Tellurium, Reprints, *Proton affinity, Oxygen atoms.

The proton affinities and structures of a series of small molecules containing group VIA atoms are calculated via ab initio electronic structure techniques. The series under study included CX, OCX, XCX, and H2CX, where X = O, S, Se, and Te. In those cases where multiple protonation sites are available, a definitive assignment of the most stable site is reported. Excellent agreement with the experimentally known proton affinities is found in almost all cases. The results indicate that the general trend which one would expect upon moving down a column of the periodic table is born out, with a particularly large change on going from the first to the second row. Calculations were performed at both the SCF and correlated levels with compact effective potentials used to replace the core electrons. Complete structural optimizations via analytic gradients were performed utilizing basis sets of at least double zeta plus polarization quality.

*600,227*
**PB86-193042** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Novel Synthesis of Methyltin Triiodide with Environmental Implications.**
Final rept.,
W. F. Manders, G. J. Olson, F. E. Brinckman, and J. M. Bellama. 1984, 3p
Pub. in Jnl. of the Chemical Society, Chemical Communications n8, p538-540 1984.

Keywords: *Tin organic compounds, *Environments, Reaction kinetics, Methylation, Reprints, *Stannanes/methyl, Stannane/methyl-triiodide, Sulfur/methyl.

Methyltin triiodide and methylsulfur species are produced by an unusual heterogeneous reaction between methyliodide with stannous sulfide in water at room temperature which may bear on ubiquitous occurrence of methylstannanes in the environment.

*600,228*
**PB86-193075** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.
**Structures and Reactions of C3H6 (1+) Ions Generated in Cyclopropane.**
Final rept.,
S. G. Lias, and T. J. Buckley. 1984, 15p
Pub. in Int. J. Mass Spectrom. Ion Processes 56, n2 p123-137 1984.

Keywords: Ionization, Isomerization, Proton affinity, Reprints, *Charge transfer, *Cyclopropane, Ion cyclotron resonance.

Ions of the formula C3H6+ have been generated by charge transfer to cyclopropane from C6F6+ (recombination energy, 9.91 eV), CS2+ (recombination energy, 10.08 eV), COS+ (recombination energy, 11.18 eV), and Xe+ (recombination energy, 12.127 eV). From a determination of the charge transfer equilibrium constant in the c-C3H6:C6F6 mixture a value for the 300 K ionization energy of cyclopropane of 9.86 eV is obtained. In addition to the characteristic CH2NH2+ and CH2NH3+ products formed in reactions of c-C3H6+ with ammonia, ions formed with no excess energy transfer a proton to ammonia. The probability of the occurrence of the proton transfer channel is about 30% for ions formed by charge transfer from C6F6+, CS2+, or COS+, but increases to 50% for ions formed by charge transfer from Xe+, which indicates that about 30% of the C3H6+ ions

formed by charge transfer from Xe+ have undergone the isomerization process: c-C3H6+-> CH3CH=CH2.

*600,229*
**PB86-193711** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Alkoxide Precursor Synthesis and Characterization of Phases in the Barium-Titanium Oxide System.**
Final rept.,
J. J. Ritter, R. S. Roth, and J. E. Blendell. 1986, 8p
Pub. in Jnl. of the American Ceramic Society 69, n2 p155-162 Feb 86.

Keywords: *Synthesis(Chemistry), *Barium, X rays, Diffraction, Reprints, Alkoxide precursors, Barium monotitanate.

Barium titanate precursors with Ba/Ti ratios ranging from 2:1 to 1:9 were prepared by controlled hydrolysis of mixed barium and titanium species in an alcohol medium. Details of the synthesis and characterization of the resultant products are given. Amorphous powders precipitated by hydrolysis from ethanol solutions of barium and titanium alkoxides crystallize to single- or two-phase 1:2 and 1:5 compounds at approximately 700 C. These compounds transform at higher temperatures to other known crystalline phases, the 1:5 phase being maintained metastably to approximately 1100 C.

*600,230*
**PB86-193927** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Study of the Collisional Activation of Cyclobutanone by the Transient Heating of Tetrafluorosilane.**
Final rept.,
M. D. Scheer, J. R. McNesby, and W. Braun. 1984, 5p
Pub. in Jnl. of Physical Chemistry 88, n9 p1850-1854 1984.

Keywords: Decomposition, Interactions, Reprints, *Tetrafluorosilane, *Cyclobutanone, Unimolecular reactions, Laser heating.

The unimolecular decomposition of cyclobutanone has been used to study the behavior of SiF4 as a heat bath gas. Temperatures in the neighborhood of 1050 K were obtained by rapid flow through a heated tube and by the absorption of the pulsed infra-red radiation emitted by a CO2 TEA laser tuned to 1033/cm. The effective reaction times of these two heating methods were approximately one millisecond and 100 microseconds respectively. The two separate decomposition channels of cyclobutanone were studied by means of a comparative method that is insensitive to the non-uniform temperatures inherent in all transient heating methods.

*600,231*
**PB86-196441** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Iodomethane as a Potential Metal-Mobilizing Agent in Nature.**
Final rept.,
J. S. Thayer, G. J. Olson, and F. E. Brinckman. 1984, 4p
Pub. in Environmental Science and Technology 18, n9 p726-729 1984.

Keywords: Chemical reactions, Environments, Metals, Sulfur organic compounds, Reprints, *Methane/iodo.

Iodomethane, an ubiquitous biogenic metabolite, has been found to release metals from polluted anoxic sediments, and also from certain metal compounds. Reactions of metal sulfides with iodomethane gave methylsulfur compounds. Kinetic investigations upon the dissolved Na2S/CH3I system, using proton NMR spectroscopy, showed a second-order reaction having the rate constant K = 0.001 L/mol.s. Naturally occurring iodomethane may react with metal sulfides or metals under certain environmental conditions to generate water-soluble and/or volatile derivatives.

*600,232*
**PB86-201431** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Solid-State 13C NMR Probe for Organotin(IV) Structural Polymorphism.**
Final rept.,
T. P. Lockhart, and W. F. Manders. 1986, 3p
Pub. in Inorganic Chemistry 25, n4 p583-585 1986.

Keywords: *Polymorphism, *Tin organic compounds, Stannates, Nuclear magnetic resonance, Crystal structure, Reprints, *Stannanes/methyl, Carbon 13.

Solid-state (13) C NMR spectra are reported for three methyltin(IV) compounds which display two types of structural polymorphism. Date for (Me2SnS)3 and Me2Sn(S2CNEt2)2, both of which are known to exist in two or more crystalline forms, demonstrate the ability of the NMR experiment to distinguish between different crystalline modifications of a single compound. The two methyl (13) C resonances in the solid-state NMR of pure, crystalline MeSnPh3 require the presence of more than one structural form in the sample; evidence is cited which indicates that MeSnPh3 adopts two forms within a single crystalline modification. General comments on the use of solid-state NMR for determining the occurrence of structural polymorphism are made.

*600,233*
**PB86-208402** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Fourier Transform Spectrum of the Torsional Band of Hydrazine.**
Final rept.,
N. Ohashi, W. J. Lafferty, and W. B. Olson. 1986, 15p
Pub. in Jnl. of Molecular Spectroscopy 117, p119-133 1986.

Keywords: Vibrations, Spectral fit, Torsional band, Infrared, Reprints, *Fourier transform, *High resolution, *Hydrazine.

The far-infrared torsional band of hydrazine has been studied by Fourier transform spectroscopy with an apodized resolution of 0.011 per cm. As a result of torsional as well as inversion tunneling, large splittings are observed in this b-type band. About 700rRk and pPk transitions of 22 subbands with delta k.k' from -10 to + 11 were assigned. The A-B, B-A, and E-E transitions were assigned for all subbands except for the delta K.K =-2 and -1 subbands, for which only the nondegenerate transitions were observed. A global fitting, which includes all available ground state microwave data, was made using Hougen's group theoretical formalism. Several fitting constants, i.e., B-C, the trans torsional tunneling constant ht3v, and the inversion tunneling constant h5v, were found to exhibit large changes upon torsional excitation. The values of these constants in the torsional fundamental state are: B-C = 184.52(30) MHz, ht3v = -912.0(21) MHz, and h5v =1994.1(16) MHz, where the numbers in parentheses are 1 O. (Copyright (c) 1986, Academic Press, Inc.)

*600,234*
**PB86-208485** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Ion Thermochemistry: Summary of the Panel Discussion.**
Final rept.,
S. G. Lias. 1984, 6p
Pub. in Ionic Processes in the Gas Phase, p355-360 1984.

Keywords: *Thermochemistry, Reprints, *Ion thermochemistry.

The Panel on Ion Thermochemistry included a discussion by Dr. Tomas Baer of the problems inherent in detecting an ionization onset, results on ionization potentials of radicals from the laboratories of Dr. J. L. Beuchamp and of Dr. J. M. Dyke (presented in his absence by S. G. Lias), new experimental data on the proton affinity scale in the region below water from Dr. T. B. McMahon, and a presentation of information about the dissociation of protonated dimers by Dr. R. E. March. In addition, Drs. S. G. Lias, J. L. Holmes, and J. E. Bartmess gave details of a comprehensive evaluation of hearts of formation of ions in progress at the time of this writing. Synopse of these presentations are given below.

*600,235*
**PB86-209160** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Solid State 13C NMR Molecular Structure of Microcrystalline, Polymeric Me2SnHPO4.**
Final rept.,
T. P. Lockhart, and W. F. Manders. 1986, 3p
Pub. in Inorganic Chemistry 25, n7 p1068-1070, 26 Mar 86.

Keywords: *Molecular structure, Nuclear magnetic resonance, Reprints, *Dimethyltin hydrogen phosphates, Carbon 13.

No abstract available.

*600,236*
**PB86-209178** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Structure Determination by NMR Spectroscopy. Correlation of (sup 2)J ((119)Sn, (1)H) and the Me-Sn-Me Angle in Methyltin(IV) Compounds.**
Final rept.,
T. P. Lockhart, and W. F. Manders. 1986, 4p
Pub. in Inorganic Chemistry 25, n7 p892-895, 26 Mar 86.

Keywords: *Molecular structure, Tin organic compounds, Nuclear magnetic resonance, Organometallic compounds, Reprints, *Stannanes/methyl, Methyltin compounds.

Isotone regression techniques are reinterpreted and extended to include upper and lower bounds on the ordered sequences in question. This amounts to solving the shortest distance problem for the order simplex (S sup n) in (R sup n). An 0(n) algorithm is presented for this problem, verified via the Kuhn-Tucker conditions, and explained geometrically in terms of the Lagrange multipliers. In this context, isotone regression techniques are interpreted in terms of orthogonal projections onto faces of the order simplex (S sup n). These projections provide a succinct characterization of the descent directions required for the design of gradient projection methods for minimizing differentiable functions on (S sup n). The latter problem arises in parameterized curve fitting. The authors conclude by considering generalizations of these techniques.

*600,237*
**PB86-232758** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Chemical Thermodynamics of Actinide Elements and Compounds. Part 8. The Actinide Halides.**
Final rept.,
J. Fuger, V. B. Parker, W. N. Hubbard, and F. L. Oetting. 1983, 267p
Pub. in Chemical Thermodynamics of Actinide Elements and Compounds. Part 8 - The Actinide Halides, 267p 1983.

Keywords: *Thermodynamics, *Actinide series, Americium, Curium, Neptunium, Plutonium, Protactinium, Uranium, Thorium, Enthalpy, Entropy, Temperature, Oxygen halides, Specific heat, Heat capacity.

Chemical thermodynamic properties of halides, oxyhalides, etc. of thorium, protactinium, uranium, neptunium, plutonium, americium and curium are reviewed, evaluated and tabulated. Properties covered are enthalpy of formation, Gibbs energy of formation, entropy, heat capacity and enthalpy, as a function of temperature.

*600,238*
**PB86-239753** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Electronic and Geometric Structures of Pt(NH3)2 (2+) Pt(NH3)2 Cl2, Pt(NH3)3 X, and Pt(NH3)2 XY (X,Y=H2O, OH(1-) ).**
Final rept.,
H. Basch, M. Krauss, W. J. Stevens, and D. Cohen. 1985, 5p
Pub. in Inorganic Chemistry 24, n21 p3313-3317 1985.

Keywords: *Molecular structure, Stereochemistry, Molecular isomerism, Ligands, Reprints, *Electronic structure, *Cis trans isomerization, *Pt diamine complexes.

Isomeric energies and conformations for Pt(NH3)2(2+) (DP), Pt(NH3)2(2+)Cl2 (DDP) Pt(NH3)3 x and Pt(NH3)2 XY (X=NH3, H20, OH-; Y=H2O, OH-) have been calculated by ab initio molecular orbital theory using energy gradient methods. The trends in metal-ligand bond lengths follow a con-

sistent pattern which permits the development of a trans influence ordering of ligands. The OH(1-) ligand is predicted to be in an unusal position in the ordering. However, the experimentally derived ordering schemes may not have been examining the bare hydroxy species, which is found to seek out hypervalent hydrogen bonded attachments. The Pt(NH3)2 2+ fragment is found to have a locally stable 'cis' conformation but the trans DP and all the trans Pt(NH3)2XY complexes with X,Y=H2O, OH(1-) are lower in energy than the cis.

*600,239*
**PB87-107942** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Spectrum and Energy Levels of Y VI.**
Final rept.,
W. Persson, and J. Reader. Jul 86, 30p
Sponsored by Department of Energy, Washington, DC. Office of Magnetic Fusion Energy.
Pub. in Jnl. of the Optical Society of America B 3, n7 p959-988 Jul 86.

Keywords: *Atomic energy levels, Atomic spectra, Excitation, Reprints, *Yttrium atoms, Ionization energy.

The spectrum of the five-times-ionized yttrium atom (Y VI), excited in a sliding-spark discharge, was studied in the 160-2500-A range. About 900 Y VI lines were classified as transitions between 101 odd and 69 even energy levels. The energy-level system established includes almost all levels of the 4s2 4p4, 4s 4p5, 4s2 4p3 4d, 5d, 5s, 6s, and 5p configurations and a number of levels of the 7s, 4f, and 4s 4p4 4d configurations.

*600,240*
**PB87-109666** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**4s2 4p-4s 4p2 and 4s2 4p-4s2 5s Transitions of Galliumlike Ions from Rb VII to In XIX.**
Final rept.,
J. Reader, N. Acquista, and S. Goldsmith. Jun 86, 5p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of the Optical Society of America B 3, n6 p874-878 Jun 86.

Keywords: *Atomic orbitals, Excitation, Atomic energy levels, Plasma radiation, Far ultraviolet radiation, Reprints, Galliumlike ions, Ionization energy.

Spectra of the galliumlike ions Rb VII-In XIX excited by low-inductance sparks and laser-produced plasmas were observed with a 10.7-m grazing-incidence spectrograph. Wavelengths for the 4s2 4p doublet P(sub 0)-4s 4p2 doublet P and 4s2 4p doublet P(sub 0) - 4s2 5s doublet S multiplets, energy levels for the 4s2 4p doublet P(sub 0), 4s 4p2 doublet P, and 4s2 5s doublet S terms, and ionization energies are given for each ion.

*600,241*
**PB87-109955** Not available NTIS
Toronto Univ. (Ontario). Dept. of Chemical Engineering and Applied Chemistry.
**Critical Review of Aqueous Solubilities, Vapor Pressures, Henry's Law Constants, and Octanol-Water Partition Coefficients of the Polychlorinated Biphenyls,**
W. Y. Shiu, and D. Mackay. c1986, 19p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n2 p911-929 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: *Solubility, *Vapor pressure, Henry's law, Physical properties, *Polychlorinated biphenyls.

Relationships between the environmentally relevant physical chemical properties of the polychlorinated biphenyls, namely, aqueous solubility, vapor pressure, Henry's law constant, and octanol-water partition coefficient are discussed. Reported experimental data are tabulated and critically reviewed. Recommended values are given for 42 of the 209 congeners; however, procedures are suggested for estimating the properties of the other congeners. Properties of mixtures are not treated.

*600,242*
**PB87-113692** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Lipid-Peroxidation Model for Halogenated Hydrocarbon Toxicity - Kinetics of Peroxyl Radical Processes Involving Fatty-Acids and Fe(111) Porphyrins.**
Final rept.,
D. Brault, P. Neta, and L. K. Patterson. 1985, 9p
Pub. in Chemico Biological Interactions 54, n3 p289-297 1985.

Keywords: *Free radicals, *Toxicity, *Porphyrins, *Iron, Chemical radicals, Carbon tetrachloride, Bromoalkanes, Chloroalkanes, Fluoroalkanes, Reprints, *Chemical reaction kinetics, Peroxyl radicals.

The toxicity of halogenated hydrocarbons is believed to originate from cytochrome-P450-Mediated generated of peroxyl radicals with subsequent attack on biological targets, especially unsaturated lipid moieties. Carbon tetrachloride and the anesthetic agent halothane (CF3CHClBr), responsible for acute or incidental toxicity, respectively, are important examples. Fe(3+)-deuteroporphyrin has been used as a model for cytochrome P450, and its reactions with the peroxyl radicals CCl3O2 radicals and CF3CHClO2 radicals, derived from carbon tetrachloride and halothane, have been reported. From a study of an extended model system, the authors wish to report rate constants for reactions of CCl3O2 radicals and CF3CHClO2 radicals with unsaturated fatty acids as well as cholesterol. Rate constants for reactions of the fatty acid peroxyl radicals with the Fe(3+)-porphyrin are also presented. The model for halogenated hydrocarbon toxicity is discussed in terms of these new findings, which represent the first quantitative kinetic approach.

*600,243*
**PB87-114922** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Elucidation of Medium Effects on Molecular Structure by Solid-State and Solution 13C NMR. Identification and X-ray Structure of the Orthorhombic Modification of Dimethyltin (4) Bis(N,N-diethyldithiocarbamate).**
Final rept.,
T. P. Lockhart, W. F. Manders, E. O. Schlemper, and J. J. Zuckerman. 1986, 5p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of the American Chemical Society 108, n14 p4074-4078 1986.

Keywords: *Molecular structure, Nuclear magnetic structure, Stannates, Tin organic compounds, Structural analysis, Crystal structure, X ray analysis, Reprints, *Tin/bis(N,N-diethyl-dithiocarbamate)-phenyl.

Solid-state and solution (13)C NMR has been used to investigate medium effects on the molecular structures of Me2Sn(acac)2(acac = acetylacetonate) and Me2Sn(S2CNEt2)2. The magnitude of the Me-Sn-Me angle in different phases is obtained from analysis of the tin-carbon J coupling (sup 3 J ((119)Sn,(13)C)) data. The Me-Sn-Me angle of Me2Sn(acac)2 changes from 180 degs in the solid state (known from X-ray) to about 158 degs in benzene and 161 degs in CDCl3 (estimated from the solution (sup 3 J ((119) Sn, (13) Cl)/values). Two explanations, that a single molecule (with Me-Sn-Me = ca. 160 degs exists in solution or that rapid conflict with the molecular structures of two X-ray characterized crystalline modifications one of which contains two symmetry-independent molecules of Me2Sn(S2CNEt2)2. The suggestion that this is a third crystalline form was confirmed by X-ray analysis. The new, orthorthombic modification (space group Pbca) of SnS4N2C12H26 has a = 9.929 (2) A,b = 31.176 (5) A,C = 12.852 (1) A,Z = 8.R was refined to 0.020. The solid-state NMR-derived estimate of the Me-Sn-Me angle, 136 degs, was confirmed by X-ray analysis 135.6 (2) degs. In solution, Me2Sn(S2CNEt2)2 appears to adopt a conformation similar to that of the orthorhombic modification described here.

*600,244*
**PB87-119616** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**New Applications of Tetracyanoethylene in Organic Chemistry.**
Final rept.,
A. J. Fatiadi. 1986, 36p
Pub. in Synthesis-Stuttgart, n4 p249-284 1986.

Keywords: *Chemical reactions, Chemical properties, Synthesis(Chemistry), Chemical reaction kinetics, Organic compounds, Reprints, *Ethylene/tetracyano.

Recent applications of tetracyanoethylene in organic chemistry are reviewed; the survey is mainly concerned with selected reactions of tetracyanoethylene which have use or potential use in organic synthesis. Among other topics, the survey includes new information on molecular complexes, solute-solvent interaction, ozonation of alkenes and acetylenes (the Criegee reaction); also dehydrogenation and tricyanovinylation reactions, and reactions of tetracyanoethylene oxide; also reactions with ketones and diketones, the synthesis of heterocycles, the cationic polymerization reaction, and industrial and analytical applications. The cycloaddition reactions and reactions of tetracyanoethylene with organometallics are not included in the survey.

*600,245*
**PB87-128435** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Substituted N,N-Dialkyl Anilines: Relative Ionization Energies and Proton Affinities through Determination of Ion-Molecule Reaction Equilibrium Constants.**
Final rept.,
S. G. Lias, J. A. A. Jackson, H. Argentar, and J. F. Liebman. 1985, 6p
Pub. in Jnl. of Organic Chemistry 50, n3 p333-338 1985.

Keywords: Anilines, Ionization potentials, Chemical reactions, Reaction kinetics, Reprints, *Aniline/N-N-dialkyl, Ion-molecule collision, Charge transfer, Proton affinity.

The relative ionization energies and proton affinities of N,N-dimethyl-, N,N-diethyl-, and N,N-di-n-propylaniline, and meta- and para-methyl substituted analogues, (as well as N,N,3,5-tetramethylaniline and 4-chloro-N,N-diethylaniline) have been determined in the gas phase through measurements of the equilibrium constants of charge transfer and proton transfer reactions in an ion cyclotron resonance spectrometer. Absolute values are assigned to the ionization energies and proton affinities generated in these experiments taking as standard an evaluated ionization (7.12 eV) and proton affinity (223.4 kcal/mol) for N,N-dimethylaniline from the literature. Further, it is demonstrated that variations in both the ionization energy and the proton affinity values upon changes in ring substitution can be predicted from the appropriate Hammett sigma-values, but not from the corresponding (sigma) (1+) values; changes brought about by differing N-substituents correlate with (sigma) sup * not equal to 1 values.

## Industrial Chemistry & Chemical Process Engineering

*600,246*
**PB86-160124** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Influence of Preparation Parameters on Internal Droplet Size Distribution of Emulsion Liquid Membranes.**
Final rept.,
G. J. Hanna, and K. M. Larson. 1985, 6p
Pub. in Industrial and Engineering Chemistry, Product Research and Development 24, n2 p269-274 1985.

Keywords: *Drops(Liquids), *Membranes, *Surface areas, Mass transfer, Sedimentation, Emulsions, Lubricating oils, X-ray analysis, Solvents, Toluene, Decanes, Reprints.

Droplet-size distributions and the corresponding surface areas for emulsions prepared for emulsion liquid membranes were measured by differential X-ray sedimentation. The water-in-oil emulsions were prepared with toluene, decane, and an isoparaffnic solvent. The surface area was measured as a function of hydrocarbon solvent, emulsifier speed, time of emulsification, and aqueous weight loading. The surface area increased with increasing speed and time of emulsification, and it decreased with aqueous weight loading. Speed, time, and weight loading were all significant at the 95% level or better. Several interactions between variables were also significant. Emulsions formed with the lube-oil base were quite viscous at high aqueous

loadings which limited the creation of surface area. Typical values of the surface area ranged from 3.0 to 8.0 cu m/cu cm of aqueous phase. The effect of surface area on mass transfer rate was demonstrated with a copper extraction system.

*600,247*
**PB86-160587** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Diffusion Model for Reversible Consumption in Emulsion Liquid Membranes.**
Final rept.,
A. L. Bunge, and R. D. Noble. 1984, 17p
Pub. in Jnl. of Membrane Science 21, p55-71 1984.

Keywords: *Mathematical models, *Diffusion, *Membranes, Emulsion, Extraction, Absorption, Solutes, Chemical reactions, Reprints.

The work extends previous diffusion models for emulsion globules in which a solute reacts with an internal reagent. The model allows for reversible consumption of the solute by the internal reagent. Local concentration of the internal reagent is nonzero and satisfies reaction and phase equilibria within the reacted zone. Predicted solute absorption rates are lower for the reversible consumption model than for irreversible models.

*600,248*
**PB86-166295** PC **A08**/MF **A01**
National Bureau of Standards, Boulder, CO. National Engineering Lab.
**Center for Chemical Engineering Technical Activities: Fiscal Year 1985.**
Research summary rept. Oct 84-Sep 85,
J. Hord. Feb 86, 170p NBSIR-85/3039
See also PB85-178069. Sponsored by National Research Council, Washington, DC.

Keywords: *Chemical engineering, *Research projects, Fluid mechanics, Thermophysical properties, Measurement.

Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1985 are summarized herein. These activities fall within the general categories of process measurement, thermophysical properties data, and chemical engineering science.

*600,249*
**PB86-185279** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Measurement of the Dielectric Constant of Slurries in Pipes.**
Final rept.,
A. K. Gaigalas, and J. R. Whetstone. 1986, 11p
Pub. in Chemical Engineering Communications 40, p85-95 1986.

Keywords: *Slurries, Pipes, Attenuation, Radio transmission, Dielectric properties, Reprints, *Dielectric constant, *Ionic conductivity.

The dielectric constant and the ionic conductivity are measured for a slurry flowing in a conducting pipe. These properties are determined from a measurement of the wavelength, frequency and attenuation of radio waves propagating inside the pipe. A mixing model is used to infer the solids fraction of the slurry.

*600,250*
**PB86-196045** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Kinetic Modeling of Hydration Processes.**
Final rept.,
P. W. Brown, J. M. Pommersheim, and G. Frohnsdorff. 1983, 16p
Pub. in Cement Research Progress 1983, p245-260.

Keywords: *Cement, *Diffusion, Growth, Hydration, Kinetics, Nucleation, Reprints.

Kinetic models that may be used for the hydration of cement compounds are discussed.

*600,251*
**PB86-196052** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Kinetic Model for the Hydration of Tricalcium Silicate.**
Final rept.,
P. W. Brown, J. Pommersheim, and G. Frohnsdorff. 1985, 7p
Pub. in Jnl. Cement and Concrete Research 15, n1 p35-41 1985.

Keywords: Growth, Diffusion, Hydration, Nucleation, Reprints, *Tricalcium silicate, Kinetics.

A kinetic model describing the hydration of C3S has been developed. The model is predicated on the assumption that the formation of a final hydrate phase initiates in transient hydrate layers which surround the anhydrous grains. The transformation results in the onset of the acceleratory period. The model predicts C-S-H formation to be controlled by interfacial processes during the acceleratory period and by diffusional processes thereafter and that the growth of particles is essentially one-dimensional throughout the course of both the acceleratory and post-acceleratory periods.

*600,252*
**PB86-197340** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Critical Point Measurements on Nearly Polydisperse Fluids.**
Final rept.,
G. Morrison, and J. M. Kincaid. 1984, 6p
Pub. in AIChE (American Institute of Chemical Engineers) Jnl. 30, n2 p257-262 1984.

Keywords: *Critical points, *Hydrocarbons, Measurements, Reprints, Van der Waals.

The critical temperatures, pressures, and volumes of several mixtures containing CO2, C2H6, C3H8, and C4H10 have been measured using a heavy walled, variable volume, cylindrical glass vessel. In each mixture the relative proportions of the three hydrocarbon solutes to one another were changed; total solute mole fraction never exceded 0.1. A detailed study of the mixture CO2 + C3H8 shows that the critical temperature exhibits a minimum at a C3H8 mole fraction of 0.0265. The mixture data is analyzed using a polydisperse model of dilute solutions.

*600,253*
**PB87-110151** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Producing Liquid-Solid Mixtures (Slushes) of Oxygen or Hydrogen Using an Auger.**
Final rept.,
R. O. Voth. Sep 85, 7p
Sponsored by National Aeronautics and Space Administration, Cocoa Beach, FL. John F. Kennedy Space Center.
Pub. in Cryogenics 25, p511-517 Sep 85.

Keywords: *Oxygen, *Hydrogen, *Augers, Cryogenics, Production, Reprints, Binary mixtures.

An auger rotating inside a brass tube refrigerated with liquid helium was used to produce liquid-solid (slush) mixtures of hydrogen and of oxygen. The auger produced small particles from the cryogens so that the resulting slush mixture could be transferred and stored. The auger could produce slush continuously in an appropriate system; it could produce slush at pressures higher than the triple point pressure of the cryogen, and the energy required to produce the slush was less than the energy required to produce slush using the freeze-thaw process.

*600,254*
**PB87-118956** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Amorphous Silicon Deposition Rates in Diode and Triode Discharges.**
Final rept.,
A. Gallagher. 1986, 6p
Sponsored by Solar Energy Research Inst., Golden, CO.
Pub. in Jnl. of Applied Physics 60, n4 p1369-1373, 15 Aug 86.

Keywords: *Silicon, Deposition, Photovoltaic cells, Electric discharges, Reprints, Amorphous materials.

The relative rates of radical deposition on discharge electrodes and substrate surfaces are calculated for two-and three-electrode discharges. The reaction rate, diffusion coefficient, screen-electrode transparency, and surface sticking coefficient are parameters in the general solution. The parameters are then chosen to describe typical silane discharges used for alpha-Si:H photovoltaic production, and the effect of screen transparency and other parameters on substrate deposition rates is evaluated. The authors then show that a measurement of deposition rate versus screen-substrate spacing in a three-electrode discharge has been misinterpreted as due to gas reactions, whereas it is primarily due to screen deposition. Finally, they note some possibilities for measuring deposition parameters and for varying the mix of depositings species.

*600,255*
**PB87-134862** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Convective Instability in Packed Beds with Throughflow.**
Final rept.,
M. C. Jones, and J. M. Persichetti. 1986, 3p
Pub. in AIChE (American Institute of Chemical Engineers) Jnl. 32, n9 p1555-1557 Sep 86.

Keywords: *Fluid flow, Instability, Convection, Porosity, Temperature distribution, Reprints.

Linear stability limits are calculated numerically for convection in fluid-saturated packed beds in horizontal layers. Subject to a destabilizing temperature gradient, the effect of a net vertical throughflow is studied for various boundary condition combinations and flow direction.

## Photo & Radiation Chemistry

*600,256*
**DE83014301** MF **A01**
Boston Univ., MA.
**Fluorescence Excitation Studies of Molecular Photoionization in External Electric Fields.**
E. D. Poliakoff, J. L. Dehmer, A. C. Parr, and G. E. Leroi. 1983, 4p CONF-830821-2
Contract W-31-109-ENG-38
International conference on vacuum ultraviolet radiation physics, Jerusalem, Israel, 8 Aug 1983.
Microfiche only, copy does not permit paper copy reproduction.

Keywords: *Nitrogen, Photoionization, Fluorescence, Excitation, Electric Fields, Cross Sections, ERDA/640303.

With molecular nitrogen used as an example, it is shown that partial photoionization cross-sections for gas samples in external electric fields can be obtained through fluorescence excitation spectroscopy. (ERA citation 08:042497)

*600,257*
**PB86-161015** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Kinetics of the Early Hydration of Tricalcium Aluminate in Solutions Containing Calcium Sulfate.**
Final rept.,
P. W. Brown, L. O. Liberman, and G. Frohnsdorff. 1984, 13p
Pub. in Jnl. of the American Ceramic Society 67, n12 p793-795 Dec 84.

Keywords: *Reaction kinetics, *Hydration, Solutions, Surface areas, Concentration(Composition), Reprints, *Tricalcium aluminate, *Calcium sulfate, Hydroxyl ions.

The rates of reaction of 3CaO:A12O3 in sulfate containing solutions was investigated. It was observed that the rates of calcium sulfoaluminate hydrate formation from a mixed solution containing calcium hydroxide and calcium sulfate are much lower than those from calcium sulfate solution. In a further experiment using sulfate solution buffered with NaOH, it was established that the kinetics of calcium sulfoaluminate hydrate formation are strongly dependent on the hydroxyl ion concentration. It was also determined that the rate of sulfate ion consumption per unit surface of 3CaO:Al2O3 is constant during the period in which a calcium sulfoaluminate hydrate is the reaction product.

*600,258*
**PB86-161064** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Accurate Quantum Yields by Laser Gain vs Absorption Spectroscopy: Investigation of Br/Br* Channels in Photofragmentation of Br2 and IBr.**
Final rept.,
H. H. Haugen, E. Weitz, and S. R. Leone. 1985, 11p
Contract NAG1-437, Grant NSF-CHE79-11340
Sponsored in part by Grant NSF-PHY82-00805. Sponsored by National Aeronautics and Space Administration, Washington, DC., and National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 83, n7 p3402-3412, 1 Oct 85.

Keywords: *Bromine, *Quantum efficiency, Reprints, *Iodine bromides, Color center lasers.

A two-laser pulse-and-probe technique is used to study photofragmentation of Br2 and IBr over the wavelength range 450-530 nm. The metastable Br(doublet P(1/2)-doublet P(3/2) transition is probed by time-resolved laser gain vs absorption spectroscopy using a tunable color center laser. The new approach to the measurement of quantum yields provides highly accurate absolute values for Br*(P1/2)production. The peak quantum yield for Br2 photodissociation is phi 87% at lambda = 500 nm. the difference between the spectral variation of phi and the total absorption spectrum characterizes the A state of bromine, which contributes 14% to the absorption spectrum at lambda = 510nm. The peak in the Br* yield from photofragmentation of IBris about 73% at lambda = 500 nm. The present absolute IBr data together with the previous molecular beam studies suggest a reassessment of the contributions of the continuum states in IBr. The laser gain vs absorption method for obtaining quantum yields is readily generalized to other atoms and molecules.

*600,259*
**PB86-187721** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Application of an InGaAsP Diode Laser to Probe Photodissociation Dynamics: I* Quantum Yields from n-and i-C3F7I and CH3I by Laser Gain versus Absorption Spectroscopy.**
Final rept.,
W. P. Hess, S. J. Kohler, H. K. Haugen, and S. R. Leone. 15 Feb 86, 7p
Contract NAG1-437, Grant NSF-CHE84-08403
Sponsored in part by Grant NSF-PHY82-00805. Sponsored by National Science Foundation, Washington, DC., and National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Chemical Physics 84, p2143-2149, 15 Feb 86.

Keywords: Photochemistry, Quantum efficiency, Aliphatic compounds, Semiconductor lasers, Photochemical reactions, Reprints, *Iodine atoms, Laser applications.

No abstract available.

*600,260*
**PB86-192978** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiolytic Studies of the Cumyloxyl Radical in Aqueous-Solutions.**
Final rept.,
P. Neta, M. Dizdaroglu, and M. G. Simic. 1984, 4p
Pub. in Israel Jnl. of Chemistry 24, n1 p25-28 1984.

Keywords: *Chemical radicals, Free radicals, Reaction kinetics, Reprints, *Pulse radiolysis, *Hydroperoxide/dimethylbenzyl.

Formation and reactions of the cymyloxyl radical in aqueous solutions were studied by steady-state and pulse radiolytic techniques. Cumene hydroperoxide reacts with e (sup minus) (sub aq) (k - 4.4 x 10 to the 9th power/Ms) to yield the cumyloxyl radical. The spectrum recorded after the pulse indicates formation of a species absorbing at 250 nm. This product was identified as acetophenone, formed by the fragmentation of the cymyloxyl radical. By comparison of the pseudo-first order rates of e (sup minus) (sub aq) decay at 600 nm with the rate of production of acetophenone at 245 nm at increasing concentrations of cumene hydroperoxide, it was possible to derive a rate constant of 1.0 x 10 to the 7th power/s for the cleavage of cumyloxyl to acetophenone and methyl radical. This value is higher than that measured previously in organic solvents, as expected. Product analysis (of acetophenone and cumyl alcohol) by HPLC permitted determination of rate constants for hydrogen abstraction by the cumyloxyl radical, in competition with the fragmentation. The rate constants for i-PrOH, EtOH, and MeOH were 9,900,000, 3,800,000, and 850,000/Ms, respectively.

*600,261*
**PB86-196516** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Variational Determination of Self-Consistent Interactions in Atomic Collisions.**
Final rept.,
D. A. Micha. 1983, 9p
Pub. in International Jnl. of Quantum Chemistry 17, p153-161 1983.

Keywords: *Particle collisions, *Atomic properties, Collisions, Reprints.

State-to-state transition amplitudes are obtained from a variational functional, for two colliding atomic systems whose states are self-consistently coupled. Specifying classical center-of-mass trajectories, the approach leads to an extension of the time-dependent self-consistent field approximation; which requires iterative solutions of equations for forward and backward motions in time. The variational procedure is described for trial wave functions and trial transition densities. It is briefly illustrated with a model of two interacting two-state atoms.

*600,262*
**PB86-202835** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Reactivities of Organic Oxygen (Oxy) Radicals.**
Final rept.,
M. G. Simic, and E. P. L. Hunter. 1984, 3p
Pub. in Proceedings of Oxygen Radicals in Chemistry and Biology, Neuherberg, Munich, Germany, July 10-15, 1983, p19-21 1984.

Keywords: *Chemical radicals, *Oxygen, *Free radicals, Reaction kinetics, Organic compounds, Peroxy radicals, Alkoxy radicals, Pulse radiolysis.

Pulse radiolytic generation of peroxy, HROO, alkoxy, HRO and aroxy, ArO radicals in aqueous and nonpolar media has been exploited in the study of the properties of these organic oxygen (oxy) radicals. Special attention has been given to the formation and radical-radical disappearance of certain aroxy radicals such as phenoxy, naphthoxy, and chromanoxy radicals. Their generation by OH, O(1-) and CO3(1-), and the simplest organic oxy radical, was compared and the advantages of using CO3(1-) for 100 percent yield of aroxy radicals pointed out.

*600,263*
**PB86-229382** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiolysis of Bromophenol Blue in Aqueous Solutions.**
Final rept.,
F. A. Rahim, S. A. Eid, N. Souka, and W. L. McLaughlin. 1986, 7p
Pub. in Jnl. of Radiation Physics and Chemistry 27, n3 p211-217 1986.

Keywords: *Radiation effects, Radiolysis, Bromine aromatic compounds, Dosimetry, Gamma rays, Reprints, *Bromophenol blue, Chemical reaction kinetics, Rate constants.

The effect of gamma radiation on the color intensity of aerated and oxygenated aqueous solution of bromophenol blue (BPB) was investigated. Ionizing radiation at increasing absorbed doses (D) brought about gradual bleaching (i.e. decrease in optical absorbance, -delta A) of bromophenol blue solutions. The molar extinction coefficients of acidic, neutral, and alkaline solutions were measured and found to be independent of temperature during spectrophotometry between 20 and 40 deg C. Aerated and oxygen-saturated acidic solutions showed a linear response (-delta A vs D) up to doses of 2.4 and 2.1 kGy, respectively. Aerated alkaline solutions on the other hand showed a linear response up to 4.8 kGy. The degree of decoloration of bromophenol blue in acidic solutions was found to decrease upon the addition of ethanol, G(-BPB) decreasing from 0.24 to 0.088 upon the addition of ethanol at a concentration of .01M. Suggestions are made for possible radiation dosimetry in the dose range (0.1-5kGy) by means of spectrophotometric analysis of absorption spectra.

*600,264*
**PB86-229390** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Response of Radiation Monitoring Labels to Gamma Rays and Electrons.**
Final rept.,
F. A. Rahim, A. Miller, and W. L. McLaughlin. 1985, 9p
Pub. in Jnl. of Radiation Physics and Chemistry 25, n4-6 p767-775 1985.

Keywords: *Dosimeters, *Labels, *Chemical indicators, Gamma rays, Electrons, Quality control, Reprints, Radiation monitoring, Radiation doses, Radiochromatography.

Many kinds of coated or impregnated reflecting papers change color or become colored by large radiation doses. Such papers or 'labels' do not generally supply dosimetry information, but may give useful inventory information, namely a visual indication of whether or not an industrial product or location has been irradiated to high doses. Tests of stability, sensitivity of ambient light, and differences in dose rate and radiation type (gamma rays and electron beams) were made on 15 kinds of labels. The results show that, for many types of indicators, diverse effects may give misleading conclusions unless countermeasures are taken. For example, some of the most commonly used labels, which contain dyes that indicate changes of pH due to release of halogen from halogenated substrates, have limited shelf life and must be protected from extreme environmental conditions.

*600,265*
**PB86-232956** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Photodissociation of Ions Generated by Soft Ionization Techniques.**
Final rept.,
M. J. Welch, R. Sams, and E. White. Apr 86, 5p
Pub. in Analytical Chemistry 58, n4 p890-894 Apr 86.

Keywords: Argon lasers, Reprints, *Photodissociation, Ion lasers, Cesium ions.

Photodissociation with visible light of ions generated by the soft ionization techniques cesium ion bombardment, field desorption, and field ionization has been demonstrated. An argon ion laser was used to irradiate ions in the first field-free region of a Mattauch-Herzog geometry mass spectrometer. Ions that dissociated in the region were detected by means of a linked scan at a constant ratio of the magnetic field to the electric field. The photodissociations of $(M+H)+$ ions from methyl red and bilirubin are used to illustrate the potential of the technique for providing structural information.

*600,266*
**PB87-105896** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiation-Induced Crosslinking of Pyrimidine Oligonucleotides.**
Final rept.,
M. Dizdaroglu, and M. G. Simic. 1985, 8p
Pub. in Radiation Physics and Chemistry 26, n3 p309-316 1985.

Keywords: *Crosslinking, *Pyrimidines, Deoxyribonucleic acids, Chromatographic analysis, Radiation chemistry, Chemical radicals, Reprints, *Thymine, *Gamma radiation, Chemical reaction mechanisms, Nucleotides.

Small oligonucleotides of thymine and cytosine form crosslinks on gamma-irradiation in N2O-saturated aqueous solution. Products of crosslinking were separated and isolated by high-performance liquid chromatography and characterized by capillary gas chromatography-mass spectrometry. Quantitative measurements revealed that approximately 50% of primary water radicals account for the crosslinking. Mechanisms of product formation are presented.

*600,267*
**PB87-105904** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiation-Induced Crosslinking of Cytosine.**
Final rept.,
M. Dizdaroglu, and M. G. Simic. 1984, 8p
Pub. in Radiation Research 100, n1 p41-48 1984.

Keywords: *Cytosine, *Crosslinking, Dimerization, Chromatographic analysis, Radiation chemistry, Gas chromatography, Chemical radicals, Reprints, *Gamma radiation, Deoxycytidine, Monophosphate/deoxycytidine.

Formation of dimers upon gamma-irradiation of cytosine, 2'-deoxycytidine and 2'-deoxycytidine-5'-monophosphate in N2O-saturated aqueous solutions was found to be a major process. Quantitative measurements revealed that more than 50% of OH adduct radicals of cytosine undergo dimerization. Derivatized dimers and monomeric products were separated and identified by combined capillary gas chromatography-mass spectrometry.

*600,268*
**PB87-106126** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Triply Differential Photoelectron Studies of Resonances in Molecular Photoionization.**
Final rept.,
J. L. Dehmer, S. H. Southworth, and A. C. Parr. 1985, 6p
Pub. in Nuclear Instruments and Methods in Physics Research B10-11, n1 p247-252 1985.

Keywords: *Molecular structure, Resonance, Excitation, Ionization, Synchrotron radiation, *Photoelectrons, Reprints.

Shape and autoionizing resonances are central to the study of molecular photoionization for various reasons, the most obvious one being that they are usually displayed prominently against nonresonant behavior in such observables as the total photoionization cross section, photoionization branching ratios, and photoelectron angular distributions. More importantly, the study of resonant features has repeatedly led to a deeper physical insight into the mechanisms of excitation, resonant trapping of the photoelectron, and decay of the excited complex that occur during the photoionization process. A major impetus has been provided in the area by the ability to freely probe resonances throughout the ionization continuum with synchrotron radiation and to perform angle-resolved photoelectron spectrometry on the ejected electrons. Selected examples will serve to illustrate the recent progress and the prospects of the stream of work.

*600,269*
**PB87-110250** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Ratio of Positron to Electron Bremsstrahlung Energy Loss: An Approximate Scaling Law.**
Final rept.,
L. Kim, R. H. Pratt, S. M. Seltzer, and M. J. Berger. 1986, 8p
Grant NSF-PHY84-20845
Sponsored by National Science Foundation, Washington, DC., Office of Naval Research, Arlington, VA., and Department of Energy, Washington, DC.
Pub. in Physical Review A 33, n5 p3002-3009 May 86.

Keywords: *Positrons, Electromagnetic radiation, Cross sections, Electrons, Kinetic energy, Bremsstrahlung, Reprints, *Electron-atom collisions, *Energy losses, EV range 10-100, EV range 100-1000, *Positron-atom collisions.

The authors have calculated the total energy loss of an incident electron or positron due to the bremsstrahlung radiation from various atoms during a scattering. The kinetic energies considered for the incident electrons and positrons were 10, 50, and 500 keV. The calculations were performed with our relativistic partial-wave multipole-expansion numerical code. The differences between the radiative energy loss of positrons and electrons are considerable and cannot be disregarded. The authors observe that the ratio of the radiative energy loss for positrons to that for electrons obeys a simple scaling law, being expressible fairly accurately as a function only of the quantity T(1)/(Z squared), where T(1) is the incident-particle kinetic energy and Z is the atomic number of the scatterer. The scaling law makes it possible to obtain the energy loss for positrons from existing electron bremsstrahlung data. The scaling is exact in the case of the point Coulomb potential, both in the classical bremsstrahlung formula and the nonrelativistic dipole Sommerfeld formula, not only for the ratio of total energy losses but also for the separate energy losses and even for the radiation energy spectrum.

*600,270*
**PB87-114948** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Stark Broadening of Singly Ionized Neon Lines.**
Final rept.,
N. Konjevic, and T. L. Pittman. 1986, 5p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 35, n6 p473-477 1986.

Keywords: Ionization, Reprints, *Line broadening, *Stark broadening, *Neon ions, Stark effect, Plasma spectroscopy.

Stark profiles of 21 Ne II lines from 10 multiplets were measured in a low-pressure, pulsed arc. An electron density of 1.4 x 10 to the 23rd power/cu m was determined by laser interferometry and an electron temperature of 28000 K was measured using relative intensities of 0 II impurity lines. These experimental data are compared with a previous experiment, with semiclassical theoretical results, and with semiempirical calculations. They agree well, within experimental uncertainties, with both the experimental and the semiclassical results. However, systematic discrepancies exist when compared with the semiempirical results and these exceed the uncertainties of both the calculation and experiments. Also, the experimental Ne II Stark widths show good agreement with a recent study of regularities in plasma-broadened spectral line widths.

*600,271*
**PB87-122750** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Enhancement of Lyoluminescence by Radiation Sensitization and Chemical Dopants.**
Final rept.,
R. E. Hanig. 1984, 3p
Pub. in International Jnl. of Applied Radiation and Isotopes 35, n10 p987-989 1984.

Keywords: Radiation chemistry, Dosimetry, Disaccharides, Reprints, *Lyoluminescence, *Trehalose, Augmentation, Chemical radiation effects.

Enhancement of the lyoluminescent effect has been accomplished by radiation sensitization of solutions of trehalose, using doses of about 30, 100, and 300 krad. The disaccharide, along with associated radiolysis products, is then recrystallized from solution. Preliminary comparison of these doped sugars with untreated sugar, irradiated at doses of 1, 5, and 10 rads, indicate they give a better signal-to-background ratio for lyoluminescence dosimetry. A promising reaction model is postulated which assumes a two-component exponential decay of light, multiplied by a first-order buildup term for the dissolving factor. The model seems to fit both the ordinary and the luminol-enhanced lyoluminescent glow-curves.

*600,272*
**PB87-128450** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Quantum Yield of Vinylidene ((3)B2) from the Vacuum UV Photolysis of Acetylene and Ethylene.**
Final rept.,
A. Fahr, and A. H. Laufer. 1986, 6p
Pub. in Jnl. of Photochemistry 34, p261-266 1986.

Keywords: *Ethylene, *Acetylene, *Vinylidene resins, Photolysis, Quantum yield, Reaction kinetics, Thermoplastic resins, Chemical radicals, Ultraviolet radiation, Reprints, *Photochemistry, Vinylidene radicals, Vinyl radicals.

The primary processes in the photodecomposition in the vacuum UV of the unsaturated hydrocarbons acetylene and ethylene have been investigated. The formation of electronically excited triplet vinylidene (H2C = C) radicals is shown to be a major process. The quantum yields of vinylidene production are equal to 0.4 and 0.75 from acetylene and ethylene respectively. Vinyl radical formation in the ethylene photolysis is discussed.

*600,273*
**PB87-130506** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Spin Dependence in Superelastic Electron Scattering from Excited Sodium.**
Final rept.,
M. H. Kelley, R. J. Celotta, and J. J. McClelland. 1986, 3p
Pub. in Proceedings of DOE (Department of Energy) Atomic Physics Program Contractors' Workshop, Boulder, CO., April 14-15, 1986, 3p.

Keywords: Excitation, *Sodium atoms, Elastic scattering, Electron scattering.

Spin asymmetries are presented for superelastic scattering of spin-polarized electrons from spin-polarized M sub L = +1 and M sub L = -1 states of the Na 3P (sub 3/2) atom. The incident energy dependence at a scattering angle of 30 degrees is shown for energies of 1.26 eV to 11.76 eV. In addition, angular dependencies over the range 5 to 40 degrees are given at 2.0 and 9.26 eV. Large differences are seen between the spin asymmetries for the two M sub L-sublevels of the excited state, with the M sub L = -1 asymmetry reaching a value of 100% at 2 eV and 35 degrees scattering angle, corresponding to pure singlet scattering.

*600,274*
**PB87-134474** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Experimental Study of Stark Broadened N II Lines from States of High Orbital Angular Momentum.**
Final rept.,
T. L. Pittman, and N. Konjevic. 1986, 6p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 36, n4 p289-294 1986.

Keywords: Atomic energy levels, Ionization, Reprints, *Nitrogen ions, *Stark broadening, *Line broadening, Plasma spectroscopy.

In the paper, the authors report experimental electron impact widths for six spectral lines belonging to 3d-4f transitions of singly ionized nitrogen. Line profiles were measured in a low pressure pulsed arc. An electron density in the range 5.9-7.5x10 to the -22nd power cc m was determined from the Stark width of the He II 4686 A line, while electron temperatures of 28,300-32,300 K were measured using relative intensities of O II impurity lines. Comparison with semiempirical theoretical results does not resolve which coupling scheme, LS or LK, is better to describe atomic states in Stark broadening calculations of certain N II lines.

*600,275*
**PB87-134680** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Angular Distribution of Fluorescence from Photoionization-Produced He(1+) (n=2).**
Final rept.,
J. Jimenez-Mier, C. D. Caldwell, and D. L. Ederer. 1986, 4p
Pub. in Physical Review Letters 57, n18 p2260-2263, 3 Nov 86.

Keywords: *Fluorescence, *Helium, Angular distribution, Excitation, Reprints, Photoionization, Synchrotron radiation.

The authors report the first measurement of the angular distribution of the 304-A He(1+) (n=2) radiation following photoionization. The distribution reflects the alignment of the ion, which is related to the fraction epsilon-sigma(2p,kd)/(sigma(2p,ks)+sigma(2p,kd)) of d component in the electron wave. The experimental angular distributions correspond to alignments of -0.62 + or - 0.03 and -0.62 + or - 0.02 at photon energies of 65.5 and 66.5 eV, respectively. These translate into ratios epsilon-0.25 + or - 0.04 and 0.25 + or - 0.03, in good agreement with close-coupling calculations.

*600,276*
**PB87-137170**
(Order as PB87-137154, PC **A04**/MF **A01**)
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.

**Absolute Isotopic Abundance Ratio and Atomic Weight of a Reference Sample of Gallium,**
L. A. Machlan, J. W. Gramlich, L. J. Powell, and G. M. Lambert. 25 Jun 86, 9p
Included in Jnl. of Research of the National Bureau of Standards, v91 n6 p323-331 Nov-Dec 86.

Keywords: *Gallium, *Chemical analysis, Atomic mass, Gallium isotopes, Mass spectroscopy, *Isotope ratio, *Reference materials, Gallium 69, Gallium 71.

An absolute value has been obtained for the isotopic abundance ratio of a reference sample of gallium (Standard Reference Material 994), using thermal ionization mass spectrometry. Samples of known isotopic composition, prepared from nearly isotopically pure separated gallium isotopes, were used to calibrate the mass spectrometers. The resulting absolute (69)Ga/(71)/Ga ratio is 1.50676 + or - 0.00039, which yields atom percents of (69)Ga=60.1079 + or - 0.0062 and (71)Ga=39.8921 + or - 0.0062. The atomic weight calculated from this isotopic composition is 69.72307 + or - 0.00013. The indicated uncertainties are overall limits of error based on two standard deviations of the mean and allowances for the effects of known sources of possible systematic error.

*600,277*
**PB87-140232** PC **A14**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Technical Activities 1986, Center for Radiation Research,**
C. E. Kuyatt. Nov 86, 313p NBSIR-86/3441
See also PB86-162211.

Keywords: *Research projects, *Radiation chemistry, *Nuclear physics, *Plasma radiation, Nuclear radiation, Laboratory equipment, Sources, Calibrating.

The report summarizes research projects, measurement method development, calibration and testing, and data evaluation activities that were carried out during Fiscal Year 1986 in the NBS Center for Radiation Research. These activities fall in the areas of atomic and plasma radiation, radiation physics, radiometric physics, radiation sources and instrumentation, ionizing radiation, and nuclear physics.

*600,278*
**PB87-148367** Not available NTIS
Argonne National Lab., IL.
**Rate Constants for Reactions of Radiation-Produced Transients in Aqueous Solutions of Actinides,**
S. Gordon, J. C. Sullivan, and A. B. Ross. c1986, 12p
Prepared in cooperation with Notre Dame Univ., IN. Radiation Chemistry Data Center. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1357-1368 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Actinide series compounds, Radiation chemistry, Chemical reactions, *Rate constants.

Rate constants have been critically compiled for reactions of ions of the actinides Am, Cf, Cm, Np, Pu, Th, and U, as well as the element Tc, in different oxidation states with various chemical species in aqueous solution. The reactants include products of the radiolysis of water (hydrated electrons, hydrogen atoms, hydroxyl radicals, hydrogen peroxide) and transient species derived from other solutes (e.g., carbonate radical). The data are useful in the estimation of migration properties of actinides, which are relevant to waste management studies.

## Physical & Theoretical Chemistry

*600,279*
**AD-A121 915/3** Not available NTIS
National Bureau of Standards (NML), Washington, DC. Molecular Spectroscopy Div.
**Time Scale and Product Energy for the IRMPD of CF2HC1 at Steady State,**
John C. Stephenson. 9 Jun 82, 3p ARO-17710.4-CH
Pub. in Jnl. of Chemical Physics, v77 n6 p3283-3284, 15 Sep 82 (No copies furnished by DTIC/NTIS).

Keywords: *Halogenated hydrocarbons, *Methanes, *Fluorides, *Chlorides, *Infrared radiation, *Carbon dioxide lasers, *Photolysis, Laser induced fluorescence, Laser beams, Photochemical reactions, Reprints, *Methane/chloro-difluoro.

No abstract available.

*600,280*
**AD-A129 931/2** Not available NTIS
Colorado Univ. at Boulder. Dept. of Chemistry.
**Excimer Laser Photolysis Studies of Translational-to-Vibrational Energy Transfer In Collisions of H and D Atoms with CO,**
Charles A. Wight, and Stephen R. Leone. 3 Dec 82, 13p ARO-18660.2-PH
Contract DAAG29-82-K-0030
Pub. in Jnl. of Chemical Physics, v78 n8 p4875-4886, 15 Apr 83 (No copies furnished by DTIC/NTIS).

Keywords: *Photolysis, *Particle collisions, *Energy transfer, Atoms, Hydrogen, Deuterium, Carbon monoxide, Excitation, Excimers, Lasers, Vibrational spectra, Reprints, Laser chemistry.

No abstract available.

*600,281*
**AD-A132 741/0** PC **A02**/MF **A01**
National Bureau of Standards (NML), Washington, DC. Polymer Science and Standards Div.
**Rigorous Bounds for the Calculated Dielectric Constants of Ferroelectric Polymers.**
Technical rept.,
Martin G. Broadhurst. Aug 83, 14p Rept no. TR-21
Contract N00014-83-F-0013
Also Pub. in Ferroelectics V49, p159-167.

Keywords: *Polymers, *Ferroelectric materials, *Dielectrics, Polyvinylidenes, Fluorides, Anisotropy, Tensors, Constants, Electric moments, Crystals, Orientation(Direction), Dielectric constants, Vinylidene fluoride polymers.

A theory is presented for calculating rigorous upper and lower bounds for the dielectric constant of a semicrystalline polymer in terms of the volume fraction of crystalline phase, the dielectric constant of the liquid phase and the anisotropic dielectric tensor of the crystalline phase. Also required are two orientation functions (cos to the 2nd power theta) and (cos to the 2nd power alpha) where theta defines the tilt of crystal lamellae and alpha the orientation of the electric moment of each crystal with respect to the measuring field. Bounds are presented for polyvinylidene fluoride for a variety of orientations.

*600,282*
**AD-A133 344/2** PC **A02**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Interaction Energy for Open-Shell Systems.**
Technical rept.,
D. B. Neumann, and M. Krauss. 1 Jul 81, 6p AFOSR-TR-83-0788
Grant AFOSR-ISSA-82-0017
Pub. in Jnl. of Chemical Physics, v75 n1 p315-319, 1 Jul 81.

Keywords: *Atomic energy levels, *Potential energy, *Ground state, Hartree Fock approximation, Damping, Nuclear shell models, Coupling(Interaction), Reprints.

General expressions necessary for direct calculation of damped multipolar atomic interaction energies are presented. The ab initio method requires the computation of the zeroth and first order wave functions of each atom and can be easily applied to the interaction of open-shell atoms. Applications of this technique are given here for the case of the dipole-dipole interaction of O ('S) with O ('S, 'D, and 3P) and, using effective core potentials, Hg ('S) with Hg ('S) with Hg ('S and 3P).

*600,283*
**AD-A137 765/4** PC **A02**/MF **A01**
Colorado Univ. at Boulder. Dept. of Chemistry.
**Laser-Induced Fluorescence Studies of Ion Collisional Excitation in a Drift Field: Rotational Excitation of N2+ in Helium,**
M. A. Duncan, V. M. Bierbaum, B. B. Ellison, and S. R. Leone. 1 Dec 83, 11p AFOSR-TR-84-0076
Contract F49620-83-C-0013
Prepared in cooperation with Joint Inst. for Lab. Astrophysics, Boulder, CO. Pub. in Jnl. of Chemical Physics, v79 n11 p5448-5456, 1 Dec 83.

Keywords: *Laser induced fluorescence, *Ions, *Nitrogen, Photochemical reactions, Drift, Tubes, Electric fields, Molecular ions, Mobility, Collisions, Excitation, Helium, Molecular states, Electron transitions, Molecular rotation, Distribution, Molecules, Reaction kinetics, Energy transfer, Reprints.

Initial results are presented for a new method of studying collisional excitation and deactivation processes of molecular ions. Translationally excited ions are prepared in the uniform electric field of a drift tube. Collisions with the inert buffer gas lead to rotational and vibrational excitation (T-V,R). Laser-induced fluorescence (LIF)is used as a direct optical probe of the internal states of N2+ using the B2 epsilon(u)(+)-X2 epsilon(g)(+) transition at 391.4 nm. In this initial experiment, rotational excitation is observed for N2+ in collisions with helium at energies up to 0.054 eV (c.m.). The rotational state distribution can be described by a Boltzmann temperature corresponding to the center-of-mass collision energy, in good agreement with theory. Approximately ten collisions or less are required to obtain full equilibration of the rotational distribution. Applications of this new technqie to the interpretation of ion-molecule reaction rates in drift tubes and to the study of ion-neutral energy transfer processes are discussed.

*600,284*
**AD-A141 636/1** PC **A02**/MF **A01**
Joint Inst. for Lab. Astrophysics, Boulder, CO.
**Vibrational Energy Disposal in Polyatomic Ion-Molecule Reactions: SF6(-) + H,D Yields SF5(-) + HF(v),DF(v),**
C. E. Hamilton, V. M. Bierbaum, and S. R. Leone. 1 Mar 84, 10p AFOSR-TR-84-0411
Contract F49620-83-C-0013
Pub. in Jnl. of Chemical Physics, v80 n5 p1831-1838, 1 Mar 84.

Keywords: *Polyatomic molecules, *Ions, *Chemical reactions, *Vibrational spectra, Hydrogen, Chemiluminescence, Afterglows, Energy transfer, Reaction kinetics, Infrared spectra, Reprints, Sulfur hexafluoride, *Hydrogen fluoride.

No abstract available.

*600,285*
**DE83007670** PC **A02**/MF **A01**
Argonne National Lab., IL.
**Structure and Conductivity of the NASICON Analog Na sub 3 SC sub 2 (PO Sub 4 ) sub 3.**
S. Susman, C. J. Delbecq, T. O. Brun, and E. Prince. 1982, 3p CONF-820508-8
Contract W-31-109-ENG-38
Spring meeting of the Electrochemical Society, Montreal, Canada, 9 May 1982, Portions are illegible in microfiche products.

Keywords: *Sodium phosphates, *Scandium phosphates, Crystal structure, X-ray diffraction, Neutron diffraction, Electric conductivity, Correlations, Experimental data, Medium temperature, High temperature, Monoclinic lattices, Hexagonal lattices, ERDA/400201.

Neutron and x-ray diffraction data of Na sub 3 SC sub 2 (PO sub 4 ) sub 3 are presented that show the transition from an ordinary-conducting, high temperature phase to a still higher temperature, superionic conducting phase. There are at least four polymorphic modifications. At room temperature, the refined neutron diffraction data confirm the Cc space group reported by Efremov and Kalinin but with a = 16.0449(24), b = 8.9225(15), c = 9.0656(13)A, beta = 126.918(21), R/sub weighted pattern/ = 17.5%, and R/sub expected/ = 7%. Between 25 exp 0 C and 64 exp 0 C, a second polymorph appears. The structure is monoclinic but has not yet been refined. At 64 exp 0 C, a third polymorph C appears. It is rhombohedral R3c. Using hexagonal axes, a = 8.9273(2), c = 22.3668A, R/sub wp/ = 6.28% and R/sub e/ = 3.83% at 100 exp 0 C. At 166 exp 0 C, the high temperature polymorph D appears. It is the superconducting phase of NASICON(Sc). It, too, is rhombohedral R3c with a = 8.9274(1), c = 22.5493(6)A, R/sub wp/ = 5.81% and R/sub e/ = 3.87% at 225 exp 0 C. The diffraction data are correlated with ionic conductivity measurements as a function of temperature. (ERA citation 08:024058)

*600,286*
**DE83008648** PC **A02**/MF **A01**

National Bureau of Standards (NML), Washington, DC.
**Effects of Resonances in Molecular Photoionization Measured with Triply Differential Photoelectron Spectroscopy.**
A. C. Parr, D. M. P. Holland, D. L. Ederer, and J. L. Dehmer. 1982, 5p CONF-820883-3
Contract W-31-109-ENG-38
International mass spectrometry conference, Vienna, Austria, 29 Aug 1982, Portions are illegible in microfiche products.
Pub. in International Journal of Mass Spectrometry and Ion Physics 46, 285-288 (1983).

Keywords: *Carbon dioxide, *Polyatomic molecules, Photoionization, Resonance, Photoelectron spectroscopy, Autoionization, Franck-condon principle, Molecules, Radicals, Molecular ions, ERDA/640304.

A variable wavelength angle resolving photoelectron spectrometer has been used to study the effects of autoionization and shape resonances upon molecular photoionization. Such resonance phenomena produce non-Franck-Condon effects in the vibrational intensity distributions and significant variations in the asymmetry parameters. Results are presented for C sub 2 N sub 2 and CO sub 2 . Constant Photoelectron Energy (CPE) spectroscopy has been performed on C sub 2 H sub 2 and spectra are shown at four kinetic energies. The information concerning energy absorption in molecules gained from these studies is discussed. (ERA citation 08:024519)

*600,287*
**DE83013583** PC **A02**/MF **A01**
Los Alamos National Lab., NM.
**Mechanism of the Optogalvanic Effect in a Hollow-Cathode Discharge.**
R. A. Keller, B. E. Warner, E. F. Zalewski, P. Dyer, and R. Engleman, Jr. 17 Jun 83, 12p UCRL-88533, CONF-830646-1
Contract W-7405-ENG-48
Optogalvanic spectroscopy and application meeting, Aussois, France, 20 Jun 1983.
Pub. in J. de Phys. Colloq. C7, 44, n11 pC7-23-c7-33 Nov 83.

Keywords: *Hollow Cathodes, *Uranium, Laser Isotope Separation, Galvanomagnetic Effect, Magneto-Optical Effects, Photoemission, Electric Discharges, Ionization, Excitation, Laser Radiation, Neon, ERDA/640301, ERDA/050503.

There are two significantly different mechanisms proposed for the origin of the optogalvanic effect in a hollow-cathode discharge: (1) laser excitation of atoms to higher electronic states leads to an increased cross section for electron impact ionization, with the result that the excited atom becomes ionized and the conductivity of the discharge increases; and (2) laser excitation of atoms to higher electronic states perturbs the equilibrium established between the electron temperature and the atomic excitation temperature. Superelastic collisions between the electrons and the laser-excited atoms restore the equilibrium, with the excess energy ending up in an increased electron temperature and therefore an increased conductivity of the discharge. Both mechanisms undoubtedly proceed simultaneously and what needs to be determined is their relative importance at different discharge conditions and different excitation conditions. This is important because laser isotope enrichment schemes have been proposed using selective excitation in a hollow-cathode discharge. In order for these schemes to work, (1) must be the predominant mechanism. We have measured the optogalvanic signal, concentration of uranium atoms, impedance of the discharge, and electron temperature as a function of the discharge current in a neon-filled uranium hollow-cathode discharge. The hollow cathode operating characteristics are used as input parameters in a simple discharge model. Predictions of electron density, changes in electron temperature, and discharge impedance compare well with experimental observations. Our model and experimental observations yield a qualitative understanding of the optogalvanic effect in a hollow-cathode discharge and estimate the relative importance of the two optogalvanic mechanisms. (ERA citation 08:039521)

*600,288*
**PB84-239995** Not available NTIS
National Bureau of Standards, Washington, DC.
**Far Infrared Laser Magnetic Resonance of Vibrationally Excited CD2.**
Final rept.,
K. M. Evenson, T. Sears, and A. R. W. McKellar. Mar 84, 7p
Sponsored in part by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of the Optical Society of America B 1, p15-21 Mar 84.

Keywords: *Deuterium compounds, Excitation, Molecular energy levels, Molecular rotation, Molecular structure, Reprints, *Far infrared spectroscopy, *Laser magnetic resonance spectroscopy, *Methylene radicals, Laser spectroscopy.

The authors report the detection of 13 rotational transitions in the first excited bending state (010) of CD2 using the technique of far-infrared laser magnetic resonance spectroscopy. Molecular parameters for this state are determined from these new data together with existing infrared observations of the nu 2 band. Additional information on the ground vibrational state (000) is also provided by the observation of a new rotational transition, and this is combined with existing data to provide a refined set of molecular parameters for the CD2 ground state. One spectrum has been observed that we assign as a rotational transition within the first excited symmetric stretching state (100) of CD2. These data will be of use in refining the structure and the potential function of the methylene radical.

*600,289*
**PB86-155587** PC **A07**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
**Standard Reference Data Publications, 1964-1984,**
J. C. Sauerwein, and G. R. Dalton. Dec 85, 147p NBS/SP-708
Supersedes PB82-134362. Also available from Supt. of Docs as SN003-003-02705-7. Library of Congress catalog card no. 85-600607.

Keywords: *Standards, Chemical properties, Physical properties, Bibliographies, Information systems, Indexes(Documentation), Computer programs, *Standard reference materials, Listings.

The National Bureau of Standards' Office of Standard Reference Data manages a network of data centers that prepare evaluated data bases of physical and chemical properties of substances. Data bases are available in printed form, on magnetic tapes and through on-line computer networks. This document provides a comprehensive list of the products available from the National Standard Reference Data System (NSRDS) for the years 1964-1984, including indexes qualified by author, material, and property terms. Ordering information and current prices can be found at the end of this document.

*600,290*
**PB86-160546** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Resonant Structure in Multiphoton Ionization of Calcium.**
Final rept.,
C. L. Cromer, and C. W. Clark. 1985, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, pL497-L500 1985.

Keywords: Reprints, *Autoionization, *Calcium atoms, *Multi-photon processes.

The authors propose a candidate mechanism for the lambda = 564.6 nm resonance in multiphoton ionization of calcium observed by Agostini and Petite.

*600,291*
**PB86-160603** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Oscillator Strength Measurements of Even-Parity Autoionizing Resonances by Combined Synchrotron Radiation-Laser-Excitation.**
Final rept.,
J. M. Bizau, F. Wuilleumier, D. L. Ederer, J. C. Keller, and J. L. LeGouet. 1985, 4p
Pub. in Physical Review Letters 55, n12 p1281-1284, 16 Sep 85.

Keywords: *Molecular energy levels, Sodium, Excitation, Oscillators, Photons, Reprints, *Autoionization, *Synchrotron radiation, *Laser spectroscopy.

The authors have obtained oscillator strengths for transitions between a laser-excited initial state and autoionizing final states. In the case of sodium, a laser was used to populate the 3p initial state, and synchrotron radiation was used to excite the autoionizing resonances. The sum of the oscillator strengths for all the observed transitions between the 2p(sup 6)3p initial-state and the 2p(sup 5)3s3p final-state configurations was found to be equal to 0.22(4).

*600,292*
**PB86-160611** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Effect of Sequence Distribution on the Miscibility of Polymer/Copolymer Blends.**
Final rept.,
A. C. Balazs, I. C. Sanchez, I. R. Epstein, F. E. Karasz, and W. J. MacKnight. 1985, 4p
Contract F49620-84-C-0051
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Macromolecules 18, n11 p2188-2191 1985.

Keywords: *Copolymers, *Solubility, *Sequencing, Blends, Binary systems(Materials), Chemical bonds, Molecular structure, Reprints, *Polymer chains, Monomers.

Previous theories describing the phase behavior of copolymer blends have ignored the sequence distribution of monomer units in the copolymer. The authors introduce a parameter, theta, that describes the binary sequence distribution of the monomers in a copolymer chain. By varying theta, the authors can describe a block, random, or alternating copolymer. It is assumed that the interaction energy between a monomer of homopolymer C and the monomer A (or B) in the copolymer AB is mediated by the nearest neighbors chemically bonded to the A (or B) structural unit. It is found that the sequence distribution may significantly affect the degree of compatibility between the polymers AB and C. For a fixed composition, there is an optimal range of theta values (or sequence distributions) for which the C/AB system is miscible.

*600,293*
**PB86-160637** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Broadening of a Valence Autoionization Resonance in Electric Fields.**
Final rept.,
D. E. Kelleher, J. F. Delpech, and J. Weiner. Oct 85, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Physical Review A 32, n4 p2230-2233 Oct 85.

Keywords: *Electric fields, Reprints, *Autoionization, Line broadening.

The authors have observed a doubly excited autoionization resonance to broaden with increasing electric field. The broadening is consistent with the quadratic field dependence predicted by a simple perturbative model, but the magnitude of the observed broadening is about four times larger than predicted. Possible reasons for the discrepancy are discussed.

*600,294*
**PB86-160645** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Selective Transport of Gaseous CO through Liquid Membranes Using an Iron (II) Macrocyclic Complex.**
Final rept.,
C. A. Koval, R. D. Noble, J. D. Way, B. Louie, and Z. E. Reyes. 1985, 6p
Pub. in Inorganic Chemistry 24, n8 p1147-1152 1985.

Keywords: *Transport properties, *Carbon monoxide, *Chemical equilibrium, *Reaction kinetics, *Complex compounds, Iron organic compounds, Membranes, Reprints, *Liquid membranes, Chemical reaction mechanisms.

The equilibrium constant and rate constants for the reversible 1:1 complexation reaction, Fe(II)(TIM)(C6H5CN)2(+2) + CO K yields Fe(II)(TIM)(C6H5CN)(C0)(+2) + C6H5CN, have been measured in benzonitrile. In CO-saturated solutions, the Fe(II) complex can be oxidized electrochemically by a CrErErCi mechanism, which allows the diffusion

coefficients of the complex and CO-adduct to be determined. The reversible complexation reaction of the Fe(II) complex with carbon monoxide affords facilitated transport of CO across benzonitrile liquid membranes. For a membrane with a thickness of about 0.072 cm, the transport rate for CO is increased by 14% over the purely diffusional rate. Since the Fe(II) complex does not bind N2, O2, CO2, or H2, the facilitated transport will be selective for CO in a variety of gaseous matricies. Selectivity is demonstrated for CO/O2 gas mixtures.

*600,295*
**PB86-160652** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Rotational Relaxation of the 00(sup 0)1 Level of CO2 Including Radiative Transfer in the 4.3 Micrometers Band of Planetary Atmospheres.**
Final rept.,
A. A. Kutepov, D. G. Hummer, and C. B. Moore. 1985, 14p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 34, n2 p101-114 1985.

Keywords: *Carbon dioxide, *Rotational relaxation, *Molecular energy levels, *Planetary atmospheres, Thermodynamics, Reprints.

Accurate numerical solutions have been obtained for a model problem of rotational relaxation within the 00(sup 0)1 or vibrational level of C(12)O2(16) accounting for the transfer of radiation in the lines of the fundamental transition 00(sup 0)1-00(sup 0)0 of the 4.3 micrometers band. Intramolecular exchange of vibrational energy with the reservoir of V sub 2 quanta and absorption of solar radiation in the 00(sup 0)1-00(sup 0)0-band are accounted for. A plane-parallel isothermal atmosphere of pure CO2 with the barometric pressure distribution and solar illumination is assumed. The line opacity is represented by nonoverlapping Voigt profiles depending on temperature and pressure. The transfer problem which is equivalent to that of a multiplet with a large number of lines with a common lower level, was solved by a generalization of the Rybicki method. Absorption of solar radiation can affect significantly the source functions of lines at the centers of the P and R branches. Deviations from rotational LTE are shown to influence the intensity and shape of the 4.3-micrometers band of CO2 in the spectra of Mars and Venus, and should be taken into account in the interpretation of the observations in which the rotational structure is resolved, especially in limb measurements, where these effects are particularly apparent.

*600,296*
**PB86-160660** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Hindered and Modulated Rotations of Absorbed Diatomic Molecules: States and Spectra.**
Final rept.,
U. Landman, G. G. Kleiman, C. L. Cleveland, E. Kuster, and R. N. Barnett. Apr 84, 14p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review B 29, n8 p4313-4326, 15 Apr 84.

Keywords: *Adsorption, *Vibrational spectra, Surface chemistry, Substrates, Diatomic molecules, Reprints, Rotational states.

The authors present results for the rotational states and spectra of adsorbed diatomic molecules whose rotations are frustrated by the interaction with the substrate, for several solvable models of the interaction potentials. For a vertical adsorption configuration, hindrance is modeled by constraining the molecular motion via an infinite conical potential well. For a horizontal adsorption configuration the infinite conical-well model as well as hindrance caused by a softer hindrance potential are studied. For both hindrance models, the authors study the effects caused by a modulation of the molecular motion due to periodic azimuthal potentials dependent upon the adsorption site symmetry and other characteristics of the adsorption system. A detailed analysis of the spectra as a function of the parameters of the models is presented, allowing us to formulate a state classification scheme and draw general conclusions with regard to the systematics of the spectra of frustrated rotations of adsorbed diatomic molecules applicable to a wide class of potentials, which could guide the analysis and interpretation of data.

*600,297*
**PB86-160678** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Flowing Afterglow Infrared Chemiluminescence Studies of Vibrational Energy Disposal in the Ion-Molecule Reactions F(-1)+HBr,DBr yields HF,DF+Br(-1).**
Final rept.,
A. O. Langford, V. M. Bierbaum, and S. R. Leone. 1985, 6p
Contract F49620-83-X-0013
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics 83, n8 p3913-3918, 15 Oct 85.

Keywords: *Molecular vibration, *Chemiluminescence, *Hydrogen fluoride, *Deuterium compounds, Reprints, *Ion molecule interactions, *Flowing afterglow infrared chemiluminescence method.

Product vibrational state distributions for the ion-molecule reactions F(-1) + HBr,DBr yields HF(nu < or =4),DF(nu < or =6) + Br(+1) are determined using the flowing afterglow infrared chemiluminescence technique. A surprisal analysis suggests that less than 5% of the product molecules are formed in nu=0. The HF distribution is somewhat hotter than that reported previously, while the DF distribution is measured for the first time. Both distributions are remarkably similar to those reported for the analogous neutral processes, which suggests that direct collisions dominate the reactive encounters despite the presence of a deep attractive well in the potential surface for the ion-molecule reactions.

*600,298*
**PB86-160694** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Competition between Photoionization and Two-Photon Raman Coupling.**
Final rept.,
G. Leuchs, G. Alber, and S. J. Smith. 1985, 2p
Pub. in Proceedings of the International Conference on Laser Spectroscopy (7th), Maui, HI., June 24-28, 1985, p216-217.

Keywords: *Photoionization, *Angular distributions, *Raman spectra, Absorption, *Laser spectroscopy.

The experiment the authors describe focusses on the intensity dependence of the photoionization process leading to the first, lowest energy electron peak, which can be reached by one-photon absorption. This bound-free transition should not show any intensity dependence apart from depletion of the bound state. In contrast to this expectation they demonstrate that a third-order process involving Raman coupling to a nearby nearly degenerate state may effectively compete with the one-photon absorption process.

*600,299*
**PB86-160702** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysical Properties Div.
**Statistical Mechanical Theory of Local Compositions.**
Final rept.,
G. A. Mansoori, and J. F. Ely. 1985, 23p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in Fluid Phase Equilibria 22, p253-275 1985.

Keywords: *Fluids, *Phase transformation, Thermodynamic properties, Mixing, Reprints, *Phase equilibrium.

The concept of local composition has received much attention during the past few years, much of which has been devoted to justifying the empirical model proposed by Wilson in 1964. In the report the concept of local composition is defined on statistical mechanical grounds and expressions relating these compositions to thermodynamic properties of equilibrium fluid mixtures are derived. In particular, different local composition approximations are presented and new approximations based on molecular theories of mixtures are derived. Sets of mixing rules consistent with these different local composition approximations result, some of which are density and temperature dependent. Also, relations for partial molar properties in terms of local compositions are derived from the Kirkwood-Buff solution theory. Finally the radius of the sphere of influence of local compositions is formulated on statistical mechanical grounds.

*600,300*
**PB86-160736** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Spin Dependence in Superelastic Electron Scattering from Na(3P).**
Final rept.,
J. J. McClelland, M. H. Kelley, and R. J. Celotta. 12 Aug 85, 4p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Physical Review Letters 55, n7 p688-691, 12 Aug 85.

Keywords: *Electron scattering, *Sodium, Reprints, *Electron-atom collisions, eV range 10-100, Laser radiation, Polarized light, Electron spin polarization.

Measurements are presented of spin asymmetries for superelastic scattering of 10-eV spin-polarized electrons from the excited Na triplet P(3/2) state created by linearly polarized laser optical pumping. Asymmetries as large as 16% are observed in scattering from a state which is not spin polarized. Results are shown both as a function of scattering angle with fixed laser polarization direction, and as a function of the laser polarization direction at a fixed scattering angle.

*600,301*
**PB86-160959** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Excitation of Laser State-Prepared Na*(3p) to Na*(3d) in Low-Energy Collisions with Na(+1): Experiment and Calculations of the Potential Curves of Na2(+1).**
Final rept.,
A. Baehring, I. V. Hertel, E. Meyer, W. Meyer, and N. Spies. 1984, 15p
Sponsored by Deutsche Forschungsgemeinschaft, Bonn-Bad Godesberg (Germany, F.R.).
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 17, p2859-2873 1984.

Keywords: *Sodium, Excitation, Reprints, *Ion-atom collisions, Sodium ions, EV range 10-100.

The authors report experimental results on Na*(3p) excitation by Na(+1) impact for collision energies E(cm)=20-47.5eV together with calculated potential energy curves for the Na(+2) molecular ion for internuclear distances R=3-40 au. The state-to-state angular differential cross section for p-> collisional excitation has been measured. The authors find a pronounced maximum for the differential cross section at a reduced scattering angle tau=260eV deg. rotational coupling is responsible for the non-adjabatic collision. The largest excitation cross section is observed when the E vector of the exciting linearly polarized laser light is almost parallel to the velocity of the incoming Na (+1) ion thus preparing 3p(sigma) orbital asymptotically.

*600,302*
**PB86-161007** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Pulse Radiolysis Study of the Leucocyanide of Malachite Green Dye in Organic Solvents.**
Final rept.,
K. Bobrowski, G. Dzierzkowska, J. Grodkowski, Z. Stuglik, and Z. P. Zagorski. 1985, 9p
Sponsored by Institut Curie, Paris (France).
Pub. in Jnl. of Physical Chemistry 89, n20 p4358-4366 1985.

Keywords: *Radiolysis, *Organic solvents, Dyes, Absorption spectra, Solutions, Reprints, *Leucocyanide, *Malachite green, Chemical reaction mechanisms.

Microsecond pulse radiolysis studies have been carried out on the leucocyanide of malachite green dye (MGCN) dissolved in either 1,2-dichloroethane, chloroform, carbon tetrachloride, acetone, cyclohexane, benzene, toluene, dimethyl sulfoxide, N,N-dimethylformamide, methanol, 2-propanol, tetrahydrofuran, dioxane, benzonitrile, or acetonitrile. The transient absorption spectra obtained in argon-saturated solutions, and with various added electron scavengers (N2O, O2, or CCl4), indicate that there are several intermediate species and radiolytic products. There is evidence for the formation of an intermediate primary radical cation (MGCN (+1)) and a triplet excited state of malachite green cyanide. The first is very fast (much shorter than

the 5.5 microseconds pulse) and the second much slower (lasting tens of microseconds after the pulse). Possible mechanisms for the fast and slow components of radiolytic dye formation are postulated.

*600,303*
**PB86-161031** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Two-Photon Absorption from a Phase-Diffusing Field.**
Final rept.,
D. S. Elliott, M. W. Hamilton, K. Arnett, and S. J. Smith. 1985, 2p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of the International Conference on Laser Spectroscopy (7th), Maui, HI., June 24-28, 1985, p212-213.

Keywords: Laser radiation, *Two photon absorption, *Sodium atoms.

Field-correlation effects are studied experimentally for the weak-field two-photon 3S-5S transition in atomic sodium in a Doppler-free configuration. A laser field with the properties of constant amplitude and diffusing phase is synthesized by applying random fluctuations to a laser beam, using phase and frequency modulators. The width measured at half maximum, of the absorption profile is found to depend on band-shape as well as band width. In particular, for a Lorentzian laser power spectrum the absorption width has four times the spectral width of the exciting field.

*600,304*
**PB86-161072** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Resonant Four-Photon Ionization of Atomic Hydrogen.**
Final rept.,
D. E. Kelleher, M. Ligare, and L. R. Brewer. 1985, 3p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and National Science Foundation, Washington, DC.
Pub. in Physical Review A 31, n4 p2747-2749 Apr 85.

Keywords: *Gas ionization, *Ionization, Stark effect, Reprints, *Hydrogen atoms, *Multi-photon processes, *Photoionization.

The authors have measured the three-photon resonant, four-photon ionization profile of atomic hydrogen. The width of the profile is large compared with the laser bandwidth, fine-structure splitting, Doppler width, and radiative and collisional rates. The shape, shift, width, and laser intensity dependence of the measured profiles are in excellent agreement with theoretical predictions.

*600,305*
**PB86-162088** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Structural Analysis of Methyltin(IV) Polymers by Solid-State 13C NMR Spectroscopy.**
Final rept.,
T. P. Lockhart, and W. F. Manders. 1985, 4p
Pub. in Jnl. of the American Chemical Society 107, n21 p5863-5866 1985.

Keywords: *Molecular structure, *Nuclear magnetic resonance, Metal containing organic compounds, Reprints, *Poly(Tin/methyl), Tin oxide/dimethyl.

High-resolution solid-state (13)C NMR analysis of 11 crystalline and amorphous polymeric methyltin(IV)s is described. Multiple Sn-methyl resonances observed for linear polymeric trimethyltin acetate and trimethylstannol indicate hindered rotation of the trigonal-planar Me3Sn group in the crystal lattice. The magnitude of J of the amorphous polymers methylstannonic acid and bis(trimethyltin) carbonate provides new insight into their bonding and structure.

*600,306*
**PB86-163441** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Thermal Conductivity of Methane for Temperatures between 110 and 310 K with Pressures to 70 MPa.**
Final rept.,
H. M. Roder. Mar 85, 24p
Pub. in International Jnl. of Thermophysics 6, n2 p119-142 Mar 85.

Keywords: *Methane, *Thermal conductivity, Measurement, Reprints, Temperature dependence, Pressure dependence.

The paper presents new experimental measurements of the thermal conductivity of methane for 14 temperatures between 110 and 310 K with pressures to 70 MPa and densities from 0 to 30 mol/L. The measurements were made with a transient hot-wire apparatus and they cover a wide range of physical states including the dilute gas, the moderately dense gas, the near-critical region, the compressed liquid states, and the vapor at temperatures below the critical temperature.

*600,307*
**PB86-163466** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Electric-Field-Induced Interferences in Autoionizing Resonances.**
Final rept.,
E. B. Saloman, J. W. Cooper, and D. E. Kelleher. Jul 85, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Physical Review Letters 55, n2 p193-196, 8 Jul 85.

Keywords: *Barium, Electric fields, Resonance, Reprints, *Autoionization.

The authors have observed the effect of electric fields on the 5d9p triplet P(1) barium resonance above the first ionization threshold. The relatively broad autoionizing level is nearly degenerate with a much narrower level of opposite parity. At moderate fields, the sharp level produces an interference dip in the broad level. At higher fields, the interference eventually gives rise to two split components. The results are in good agreement with a nonperturbative theory, summarized in the Letter.

*600,308*
**PB86-163482** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Ab Initio Calculations of Radiative Transition Probabilities in SH, SH(+) and SH(-).**
Final rept.,
J. Senekowitsch, H. J. Werner, P. Rosmus, E. A. Reinsch, and S. V. O'Neil. 1985, 7p
Sponsored by National Science Foundation, Washington, DC., and Deutsche Forschungsgemeinschaft, Bonn-Bad Godesberg (Germany, F.R.).
Pub. in Jnl. of Chemical Physics 83, n9 p4661-4667, 1 Nov 85.

Keywords: *Hydrogen sulfide, Calculations, Reprints, *Radiative transition probabilities, Ab initio.

Potential energy and dipole moment functions for the ground states of SH, SH(+), and SH(-) have been calculated from highly correlated electronic wave functions. The electric dipole moments in the vibrational ground states of 32SH, 32SH(+), and 32SH(-) are calculated to be 0.74, 1.29, and 0.27 D. The predicted transition probabilities between the low lying vibrational states of the electronic ground state of SH and SD are among the smallest so far known for dipole allowed rotation-vibration transitions. The calculated A-X transition probabilities in SH confirm recent indirect determinations of the radiative lifetimes and absorption oscillator strengths in the predissociating v=0 level of the A state.

*600,309*
**PB86-163540** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Pressure Broadening, Lineshapes, and Intensity Measurements in the 0 yields 2 Band of NO.**
Final rept.,
A. S. Pine, A. G. Maki, and N. Y. Chou. 1985, 15p
Grant NSF-CHE82-19255
Sponsored by National Aeronautics and Space Administration, Washington, DC., and National Science Foundation, Washington, DC.
Pub. in Jnl. of Molecular Spectroscopy 114, p132-147 1985.

Keywords: *Nitrogen oxide(NO), Band spectra, Molecular spectroscopy, Infrared radiation, Absorption spectra, Line width, Pressure, Intensity, Reprints.

Lineshape and intensity measurements were made on the overtone band (upsilon = 2 <- 0) of nitric oxide (NO) using a tunable difference-frequency laser system. Self- and N2-pressure broadening coefficients were obtained at 296 K, and a small amount of collisional, or Dicke, narrowing (which reduces the Doppler width by about 9% at 50 Torr) was also evident. The pressure broadening observed for the doublet Pi(3/2) transitions was larger than that of the doublet Pi(1/2) for corresponding J by about 7%, so an empirical scaling law model was fit to the broadening coefficients to determine the role of interstate(spin-flipping) collisions.

*600,310*
**PB86-163557** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Self-Broadening in the Fundamental Bands of HF and HC1.**
Final rept.,
A. S. Pine, and A. Fried. 1985, 15p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Molecular Spectroscopy 114, p148-162 1985.

Keywords: *Hydrogen chloride, *Hydrogen fluoride, *Band spectra, Molecular spectroscopy, Infrared radiation, Reprints, Self broadening, Laser spectroscopy.

Self-broadened lineshapes in the fundamental bands of HF and HCl have been measured with a high-resolution difference-frequency laser spectrometer. Self-induced broadenings, shifts, and collisional narrowings have been extracted by least- squares fitting several collisional profiles to the spectra. At low pressures, the collisional narrowing effect causes deviations of the lineshapes from the Voigt profile having a Doppler-fixed Gaussian component, and yields a measure of the diffusion constants of the molecules.

*600,311*
**PB86-163581** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Absorption and Emission of Radiation in the Region of an Avoided Level Crossing.**
Final rept.,
M. O'Callaghan, A. Gallagher, and T. Holstein. 1985, 15p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review A: General Physics 32, n5 p2754-2768 Nov 85.

Keywords: Line width, Absorption spectra, Emission spectra, Band spectra, Cesium, Reprints, *Atom collisions, Atom-atom collisions, Excimers.

The spectrum for absorption and emission of radiation by colliding atoms or a diatomic molecule is calculated for spectral regions dominated by an avoided level crossing. Example processes are absorption during an atom-atom collision with separation to either crossing atomic state, total absorption to both crossing states, and spontaneous emission during a collision with either state initially populated. Absorption and emission by bound diatomic molecules (including photodissociation) is described by the theory, and as an example it is applied to the Cs2 A-X band. The authors conclude that measurements of spectra in the region of level crossing is a very powerful diagnostic of the potentials and transfer probability in the level-crossing region, which is responsible for most inelastic atom-atom energy-transfer processes.

*600,312*
**PB86-163599** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Infrared Spectrum and Autodetachment Dynamics of NH(-).**
Final rept.,
D. M. Neumark, K. R. Lykke, T. Andersen, and W. C. Lineberger. 1985, 10p
Grants NSF-PHY82-00805, NSF-CHE83-16628
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 83, n9 p4364-4373, 1 Nov 85.

Keywords: *Infrared spectroscopy, Reprints, *Autodetachment dynamics, *Negative ions.

The infrared vibration-rotation spectrum of NH- has been obtained by autodetachment spectroscopy in a coaxial laser-ion beam spectometer. Transitions from the v=0 to v=1 vibrational levels were excited with an F-center laser, and subsequent autodetachment from the v=1 levels was observed. The apparatus resolution was better than 20 MHz, allowing the resolution of the fine structure and Lambda-doubling transitions. The linewidths of the autodetachment resonances revealed some of the dynamics of the autodetachment process. The autodetachment rates were, in general, much greater for the upper Lambda-doublet levels of NH-(v=1) than for the lower levels. In addition, the increase of the autodetachment rate with rotational energy for the upper levels was much faster than would be predicted if vibrational autodetachment were the primary detachment mechanism. It therefore appears that rotational-electronic coupling plays an important role in this system, and the differences in the Lambda-doublet autodetachment rates are explained in terms of this mechanism.

*600,313*
**PB86-164381** PC **A06**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Technical Activities 1985, Molecular Spectroscopy Division,**
A. Weber. Jan 86, 110p NBSIR-86/3313

Keywords: *Molecular spectroscopy, Resolution, Research projects, Frequency standards, Photochemical reactions, Quantum chemistry, Laser applications.

The report summarizes the technical activities of the NBS Molecular Spectroscopy Division during the Fiscal Year 1985. The activities span experimental and theoretical research in high resolution molecular spectroscopy, quantum chemistry and laser photochemistry, and include the development of frequency standards, critically evaluated spectral data, applications of spectroscopy to important scientific and technological problems, and the advancement of spectroscopic measurement methods and techniques.

*600,314*
**PB86-164498** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**CO Chemisorption on Cr(110): Evidence for a Precursor to Dissociation.**
Final rept.,
N. D. Shinn, and T. E. Madey. 1 Dec 85, 17p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Jnl. of Chemical Physics 83, n11 p5928-5944, 1 Dec 85.

Keywords: *Carbon monoxide, *Chemisorption, *Chromium, Catalysis, Desorption, Reprints, Electron spectroscopy.

High resolution electron energy loss spectroscopy (EELS), electron stimulated desorption ion angular distributions (ESDIAD), low energy electron diffraction (LEED), and Auger electron spectroscopy (AES) have been combined to study CO chemisorption on the Cr(110) surface. The implications of these results to catalytic reactions of CO are considered, and comparisons to CO adsorption on clean and 'promoted' transition metals are made.

*600,315*
**PB86-164522** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Instrumentation for Photon Stimulated Desorption.**
Final rept.,
R. Stockbauer. 1984, 7p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Nuclear Instruments and Methods in Physics Research 222, p284-290 1984.

Keywords: *Surfaces, *Desorption, Reprints, *Photon stimulated desorption, Instrumentation.

Photon stimulated desorption (PSD) refers to the ejection of ions, atoms, or molecular fragments from a surface initiated by the adsorption of single photons; to date, most studies have concentrated on the detection of ions. The properties of PSD which make it attractive as a surface characterization tool are its extreme surface sensitivity, the ions being ejected only from the topmost layer and the rapidity with which the ions are ejected. Since the desorption is fast (about 10 to the -14th power s), with respect to molecular vibrations (about 10 to the -12th power s), the ion trajectory reflects the initial bonding geometry of the particle to the surface. To study the ion desorption process, one would like to measure the mass, kinetic energy distribution, angular distribution and the yield (desorption rate vs photon energy) of the desorbing ions. Time-of-flight analyzers measure only ion mass and yield, while most electrostatic deflection analyzers measure kinetic energy and yield. The ellipsoidal mirror analyzer is unique, in that it measures all four quantities simultaneously.

*600,316*
**PB86-164548** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Coriolis-Induced Intramolecular Vibrational Energy Flow between Anharmonic Normal Modes.**
Final rept.,
T. Uzer, G. A. Natanson, and J. T. Hynes. Nov 85, 7p
Sponsored by National Science Foundation, Washington, DC., and Petroleum Research Fund, Washington, DC.
Pub. in Chemical Physics Letters 122, n1-2 p12-18, 29 Nov 85.

Keywords: Energy flow, Reprints, *Intramolecular energy flow, *Coriolis coupling.

The classical flow of energy between anharmonic normal vibrational modes induced by Coriolis coupling is studied for a simple model of a linear triatomic molecule rotating in a plane. The dynamics are analytically solved via a mapping onto a hindered rotor representation. The theory is confirmed by trajectory calculations.

*600,317*
**PB86-166733** PC **A06**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Technical Activities 1985, Surface Science Division,**
C. J. Powell. Jan 86, 123p NBSIR-86/3304
See also PB81-158719.

Keywords: *Surface chemistry, Standards, Catalysis, Electron spectra, Atomic structure, Adsorption.

The report summarizes technical activities of the NBS Surface Science Division during Fiscal Year 1985. These activities include surface-standards work, experimental and theoretical research in surface science, the development of improved measurement methods, and applications to important scientific and national problems. A listing is given of publications, talks, professional committee participation, and professional interactions by the Division staff.

*600,318*
**PB86-182300** PC **A06**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Introduction to Fourier Transform Spectroscopy,**
J. Cohen. Mar 86, 102p NBSIR-86/3339

Keywords: *Infrared spectroscopy, *Chemical analysis, Spectrophotometry, Sampling, *Fourier transform spectroscopy.

The document is a simplified, concise introduction to Fourier Transform spectroscopy. The emphasis is on concepts and comprehension, and abundant diagrams are provided as an aid. The work is organized into three parts: first, a selective, but adequate review of Fourier transform mathematics, next, a treatment of the physics of a simple Michelson interferometer, and last, salient topics in Fourier transform spectroscopy.

*600,319*
**PB86-185287** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Generalized Internal Axis Method for High Barrier Tunneling Problems, as Applied to the Water Dimer.**
Final rept.,
J. T. Hougen. 1985, 32p
Pub. in Jnl. of Molecular Spectroscopy 114, p395-426 1985.

Keywords: *Water, Molecular vibration, High resolution, Reprints, Molecular rotation, Rotational states, Coordinates, Molecular tunneling.

When more than one large-amplitude vibrational motion is present in a molecule, it is often not possible to define a global internal-axis-method (IAM) coordinate system and set of basis functions. In the present work, a method is presented for extending the IAM treatment to tunneling problems in such cases, using as an illustration a model for the water dimer with three large-amplitude vibrational coordinates. The method involves the construction of two different sets of local IAM-like coordinate systems. The first of these contains n coordinate systems, one for the small neighborhood surrounding each of the n equilibrium frameworks. The second contains on the order of (n square)/2 coordinate systems, one for each feasible tunneling path between each pair of frameworks. Basis functions written in the second set of local IAM-like coordinates are used to determine the complex phase factors associated in this method with tunneling matrix elements of the phenomenological rotational Hamiltonian in the high barrier limit. These phase factors govern the way in which the various real tunneling frequencies in the molecule constructively and/or destructively interfere in the Hamiltonian matrix elements and final energy expressions.

*600,320*
**PB86-185840** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Effect of Water Loss on the Heat Capacity of Coal.**
Final rept.,
R. A. MacDonald, J. E. Callanan, and S. A. Sullivan. 1985, 8p
Pub. in High Temperatures - High Pressures 17, n3 p387-394 1985.

Keywords: *Specific heat, *Bituminous coal, *Coal, Water loss, Mathematical models, Moisture content, Reprints, Char, Volatile matter.

The moisture content of coal has a serious effect on its measured heat capacity. Measurements on high-volatile bituminous coal samples from Colorado (PSOC-854), using a differential scanning calorimeter over the temperature range 300-500 K, show that moisture evolves from apparently dried coals over a considerable range of temperature above 373 K. Recently, Merrick has developed a model to predict the loss of volatile matter from coal, the resulting heat capacity of the char, and the heat loss due to the evolution of volatile components, for temperature above 573 K. At the lower temperatures used in the experiments reported here, water is the only component that evolves, and Merrick's model has been adapted to this situation. The results of the calculation of the heat capacity are presented and compared with experimental values.

*600,321*
**PB86-186699** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Photoeffect in the 4d Subshell of Atomic Silver Between 14 and 140 eV.**
Final rept.,
M. O. Krause, W. A. Svensson, T. A. Carlson, G. Leroi, and D. E. Ederer. 1985, 7p
Contract DE-AC05-84OR21400
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, p4069-4075 1985.

Keywords: Cross sections, Palladium, Reprints, *Silver atoms, *Photoelectron spectroscopy, *Photoionization, EV range 10-100, EV range 100-1000.

Relative partial photoionisation cross sections and the photoelectron angular distribution parameter beta have been measured for the 4d electrons of atomic silver in the energy range 14 = or < h(nu) = or <140 eV. Data are found to be in good agreement with the results calculated in the relativistic random-phase approximation (RRPA) for the neighbouring atom palladium. Comparison with solid-state data reveals a dominant atomic character of the 4d electrons in metals. This is especially evident for the beta parameter. However, differences occurring around the Cooper minimum at 130 eV show the influence of the metallic state on the properties of the 4d electrons.

*600,322*
**PB86-186723** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

**Copolymer/Copolymer Blends: Effect of Sequence Distribution on Miscibility.**
Final rept.,
A. C. Balazs, F. E. Karasz, W. J. MacKnight, H. Ueda, and I. C. Sanchez. 1985, 3p
Contract F49620-84-C-0051
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Macromolecules 18, n12 p2784-2786 1985.

Keywords: *Copolymers, *Solubility, Interactions, Blends, Distribution(Property), Chemical composition, Reprints.

An earlier theory on the effect of sequence distribution in copolymer/homopolymer blends is applied to blends of two copolymers that differ only in composition. A general expression for (chi blend) is derived which contains contributions from a composition dependent term (Chi comp), as well as a term (Chi dist) which depends only on the difference between the sequence distributions in the two copolymers. A special case of the above equation is a blend where both copolymers have the same composition but differ only in sequence distribution: for example, a blend of a 50:50 alternating copolymers with a 50:50 random copolymer. The general formula is adapted to the case, and the authors can theoretically confirm the experimental observation that PVC and chlorinated polyethylene (CPE) of the same composition are immiscible. From experimental data on CPE/CPE mixtures, they can evaluate the chi parameters required by their theory and consequently calculate (chi sub CH2; CHC1.)

*600,323*
**PB86-186731** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**H2O Adsorption on Oxygen-Dosed Ni(110) - Formation and Orientation of OH(ad).**
Final rept.,
C. Benndorf, C. Nobl, and T. E. Madey. 1984, 13p
Pub. in Surface Science 138, n2-3 p292-304 1984.

Keywords: *Surface chemistry, *Water, *Nickel, Orientation, Adsorption, Reprints, *Hydroxyl radicals, Electron stimulated desorption.

The presence of oxygen on a Ni(110) surface promotes the adsorption and decomposition of H2O at 300 K. Angle resolved UPS (ultraviolet photoemission spectroscopy), ESDIAD (electron stimulated desorption ion angular distribution) and isotope experiments all indicate that OH(ad) is formed on the surface, presumably via a hydrogen abstraction reaction, H2O + O(ad) -> 2OH(ad). The molucular axes of the OH(ad) species are inclined with respect to the surface normal, and are oriented along (001) and (001) azimuthal directions.

*600,324*
**PB86-186749** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Mass Spectrometry of 2-Substituted-4-Arylthiazoles. 3. Identification of Microsomal Nitroreduction Products by Mass Spectrometry.**
Final rept.,
M. B. Mattammal, T. V. Zenser, B. B. Davis, and E. White. 1984, 6p
Sponsored by Veterans Administration Medical Center, Washington, DC., and Saint Louis Univ., MO.
Pub. in Biomedical Mass Spectrometry 11, n4 p149-154 1984.

Keywords: *Thiazoles, Chemical reactions, Mass spectroscopy, Heterocyclic compounds, Carcinogens, Nitro compounds, Reduction, Reprints, Thiirene/phenyl.

The electron impact mass spectra of the chemical carcinogens 4-(4-nitrophenyl)-2-methylaminothiazole, 4-(4-aminophenyl)-2-methylaminothiazole and 4-(4-aminophenyl)-2-aminothiazoles were studied. The 4-(4-aminophenyl)-2-substituted thiazoles were isolated from the anaerobic microsomal reduction of their respective 4-nitrophenyl analogues. The identity of the reduction products were established by chemical synthesis and mass spectrometry. The mass spectrometric fragmentation of the nitro derivative shows prominent ions arising from the loss of the nitro group, ring enlargement of the thiazoles, and the phenylthiirene ion resulting from 1,2-cleavage of the thiazole ring. In the 4-(4-aminophenyl)-2-substituted amino derivative prominent ions result from the preferential 1,2-cleavage of the thiazole ring to give the common 2-(4-aminophenyl)thiirene ion and subsequent fragmentation of the ion.

*600,325*
**PB86-186764** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Methylthiirane: Kinetic Gas-Phase Titration of Sulfur Atoms in (SxOy) Systems.**
Final rept.,
R. I. Martinez, and J. T. Herron. 1983, 6p
Pub. in International Jnl. of Chemical Kinetics 15, n11 p1127-1132 1983.

Keywords: *Reaction kinetics, *Sulfur oxides, Gases, Titration, Reprints, *Methylthirane, *Sulfur atoms.

The reaction SO + SO ->S + SO2 was studied in the gas phase at 298 K by using methyl thiirane as a titrant for sulfur atoms. By monitoring the C3H6 produced in the reaction S + CH3-CH-CH2-S-> S2 + C3H6, the authors determined an expression for (K sub 2). (K sub 2) approx = (10 to the power (-12.0 + or -0.3))(e exp (-1700 + or - 200))/T cc/s, (T = 298-1000K).

*600,326*
**PB86-187036** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Formulations for the Thermodynamic Properties of the Saturated Phases of H2O from 173.15 K to 473.15 K.**
Final rept.,
R. W. Hyland, and A. Wexler. 1983, 20p
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 89, Pt. 2A/2B p500-519 1983.

Keywords: *Thermodynamic properties, *Water, *Ice, *Water vapor, Enthalpy, Entropy, Vapor pressure, Reprints.

No abstract available.

*600,327*
**PB86-187044** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Dependence of the Stimulated Emission Cross Section of Yb(3+) on Host Glass Composition.**
Final rept.,
M. J. Weber, J. E. Lynch, D. H. Blackburn, and D. J. Cronin. Oct 83, 9p
Sponsored by Lawrence Livermore National Lab., CA.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Jnl. of Quantum Electron QE-19, n10 p1600-1608 Oct 83.

Keywords: Laser materials, Cross sections, Fluorescence, Glass, Reprints, *Ytterbium ions, *Stimulated emission.

The stimulated emission cross section for the doublet F (5/2) -> doublet F (7/2) transition of Yb(3+) has been determined from absorption and emission measurements of 41 different oxide, fluoride, and oxyfluoride glasses at 293 K. The effective peak cross sections for transitions to Stark levels above the ground state range from approximately 0.3 to 0.8 pm sup 2. The largest values occur in borate and phosphate glasses; the smallest values occur in silicate and low-refractive-index fluoride glasses. Radiative lifetimes calculated from integrated absorption spectra are also reported and range from 0.6 to 2.7 ms. Systematic variations in cross sections with changes in modifier ions can be used to tailor stimulated emission cross sections and fluorescence lifetimes.

*600,328*
**PB86-187101** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Characterization of Organometallic Polymers by Size Exclusion Chromatography on Preconditioned Columns.**
Final rept.,
E. J. Parks, W. F. Manders, R. B. Johannesen, and F. E. Brinckman. 1986, 13p
Sponsored by David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.
Pub. in Jnl. of Chromatography 351, p475-487 1986.

Keywords: *Chromatographic analysis, *Polymers, Tin organic compounds, Chemical analysis, Reprints, *Chemical reaction mechanisms.

Tin-bearing organometallic polymers (OMPs) having tributyltin substituents on pendant carboxylic acid groups are in current, extensive use as marine biocides. Fractionation of the substituted polymer by size exclusion chromatography (SEC) on polystyrene cross-linked with divinylbenzene (PS-DVB) is complicated by surface adsorption of cations even on this relatively inert packing material. The paper describes chromatography performed successfully on PS-DVB columns following pretreatment with an organometallic cation to establish a positively charged surface. Tin-specific SEC illustrates the methodology. The column packing is preconditioned with an organic solution of tributyltin-bearing cation derived from monomer esters, to prevent cleavage of the tin-bearing moieties from the OMP. Mass-sensitive differential refractive index and element-specific graphite furnace atomic absorption spectroscopy detectors in tandem give self-consistent values for key molecular parameters (molecular weight, molecular weight dispersion, and the distribution of tin in high- and low-molecular-weight fractions).

*600,329*
**PB86-187119** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Static and Kinetic Studies of Polystyrene/Poly(vinylmethylether) Blends.**
Final rept.,
C. C. Han, M. Okada, Y. Muroga, F. L. McCrackin, and B. J. Bauer. 1986, 6p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Polymer Engineering and Science 26, n1 p3-8 Jan 86.

Keywords: *Reaction kinetics, Static characteristics, Interactions, Thermodynamic properties, Vinyl ether resins, Polystyrene, Phase diagrams, Reprints, Spinodal decomposition.

A systematic study of static and kinetic phase behavior of deuterated polystyrene/poly(vinylmethylether) blends is presented in the paper. The static properties are studied by the small angle neutron scattering techniques and the kinetics of phase decomposition are studied by the temperature jump light scattering technique. The procedure provides detailed information about phase behavior with regard to both thermodynamics and kinetics.

*600,330*
**PB86-187127** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Precision Measurement of the 1s Lamb Shift in Hydrogenlike Argon.**
Final rept.,
E. S. Marmar, J. E. Rice, E. Kaellne, J. Kaellne, and R. E. LaVilla. 1986, 4p
Grant DE-AC02-78ET1013
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A: General Physics 33, n1 p774-777 Jan 86.

Keywords: Argon, Wavelengths, Emission spectra, Accuracy, Calibrating, Measurement, Reprints, *Argon plasma, *Lamb shift, Alcator device.

Precision measurements of the absolute wavelengths of the Lyman-alpha doublet (2p doublet P(3/2,1/2)->5s doublet 5(1/2)) in hydrogenlike argon Ar(+17), as well as those of some strong dielectronic satellites, are reported. The Alcator C tokamak plasma was seeded with trace amounts of argon and the emission spectra were taken with a high-resolution, crystal x-ray spectrometer. In situ wavelength calibration was achieved by utilizing the potassium K alpha lines from a KCl fluorescence source. For the Ly alpha sub 2 line, a precision of 11 ppm was achieved. Comparisons of these data with QED predicted wavelengths show good agreement, yielding a test of the 1s Lamb shift at the 3% level. The precision of these measurements was limited by uncertainties in the wavelength calibration, with the uncertainties due to the influence of unresolved satellites being of secondary importance.

*600,331*
**PB86-187135** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

**Charge Transfer and Vibrational Excitation in Molecule-Surface Collisions: Trajectorized Quantum Theory.**
Final rept.,
J. W. Gadzuk, and S. Holloway. 1985, 10p
Pub. in Physica Scripta 32, p413-422 1985.

Keywords: *Surfaces, Diatomic molecules, Excitation, Molecular vibration, Iodine, Nitrogen, Quantum theory, Reprints, *Charge transfer, Molecule-molecule collisions, Molecular trajectories, Molecular ions.

Vibrational excitation of diatomic molecules scattered from solid surfaces is considered. Emphasis is placed on a mechanism in which charge transfer between the molecule and surface creates a temporary molecular ion. A classical mechanics analysis of the effect has been presented previously. Here a mixed picture is offered in which the center-of-mass translational motion is treated classically with a trajectory approximation (TA) and the intramolecular vibrational motion quantum mechanically. A procedure for insuring energy conservation and microscopic reversibility in the TA is given. Both state-to-state T->V probabilities and mean energy transfer to the vibrational system are calculated for parameters which model N sub 2 and I sub 2 molecules and the results are considered in the light of the 'exact' classical mechanics results.

*600,332*
**PB86-187259** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Comparison of Vibrational Broadening in Auger and Photoelectron Spectroscopy.**
Final rept.,
J. A. D. Matthew. 1984, 4p
Pub. in Physical Review B 29, n6 p3031-3034, 15 Mar 84.

Keywords: *Surfaces, Rare gases, Metals, Adsorption, Reprints, *Photoelectron spectroscopy, *Auger electron spectroscopy.

Within linear coupling the vibrational broadening of quasi-atomic Auger peaks and core photoelectron peaks is approximately equal in ionic crystals, but the Auger Broadening is about three times that of the core photoelectron broadening for rare gas atoms physisorbed on metal surfaces.

*600,333*
**PB86-187275** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Molecular Symmetry and Translation-Rotation Coupling In Orientationally Disordered Crystals.**
Final rept.,
K. H. Michel, and J. M. Rowe. 1 Nov 85, 8p
Sponsored by Institut Interuniversitaire des Sciences Nucleaires, Brussels (Belgium).
Pub. in Physical Review B 32, n9 p5818-5826, 1 Nov 85.

Keywords: *Phase transformations, Degrees of freedom, Crystal symmetry, Reprints, Ferroelasticity.

The theory of coupling between rotational and translational degrees of freedom in orientationally disordered crystals is studied in detail, with careful attention to the requirements of symmetry. An essential feature of this coupling is the presence or absence of a center of symmetry in the molecule or molecular ion, which determines the nature of the coupling to optic- and acoustic-phonon modes. The present analysis is relevant for the understanding of ferroelastic phase transitions, of incommensurate transitions in insulators, and of structural transitions and related properties in synthetic organic conductors.

*600,334*
**PB86-187283** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Aqueous Solubilities, Octanol Water Partition Coefficients, and Entropies of Melting of Chlorinated Benzenes and Biphenyls.**
Final rept.,
M. M. Miller, S. Ghodbane, S. P. Wasik, Y. B. Tewari, and D. E. Martire. 1984, 7p
Pub. in Jnl. of Chemical Engineering 29, n2 p184-190 1984.

Keywords: *Chemical analysis, *Chlorobenzenes, *Biphenyl/perchloro, Solubility, Entropy, Chlorine organic compounds, Reprints, Partition coefficients.

The aqueous solubilities and octanol/water partition coefficients at 25 C are determined for 12 chlorobenzenes, 16 polychlorinated biphenyls and for biphenyl using the modified generator column method. These values are correlated with chlorine number and with either boiling point for the chlorobenzenes or the relative retention time of a polychlorinated biphenyl eluting from a gas chromatographic column. Using differential scanning calorimetry, the melting points and enthalpies of melting for those compounds which are solid at room temperature are determined. A correlation between the octanol/water partition coefficient and corrected aqueous solubility is also presented, and the universality of the derived eqation is demonstrated.

*600,335*
**PB86-187291** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**FT-IR (Fourier Transform Infrared) Microspectroscopic Method for Kinetic Measurements at High Temperatures and High Pressures.**
Final rept.,
P. J. Miller, G. J. Piermarini, and S. Block. 1984, 7p
Sponsored by Naval Surface Weapons Center, Silver Spring, MD.
Pub. in Applied Spectroscopy 38, n5 p680-686 1984.

Keywords: *Reaction kinetics, Pyrolysis, Infrared spectroscopy, Reprints, Fourier transform spectroscopy, RDX, Pressure dependence, Temperature dependence.

A Fourier transform infrared microspectroscopic method has been developed for obtaining kinetic data as a function of pressure and temperature. The method employs a diamond anvil high pressure cell with heating capability in conjunction with a FT-IR spectrometer modified with an on-axis cassegrain-type beam condenser. Time-dependent absorption spectra have been obtained for the thermal decomposition of 1,3,5-Trinitrohexahydro-1,3,5-Triazine (RDX) as a function of pressure and temperature. The pressure dependence of the temperature of thermal decomposition has also been determined. The method has wide applicability to kinetic measurements in general.

*600,336*
**PB86-187671** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Interactions of CO + K on Ru(001): Structure and Bonding.**
Final rept.,
T. E. Madey, and C. Benndorf. 1985, 23p
Sponsored by North Atlantic Treaty Organization, Brussels (Belgium), and Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Surface Science 164, p602-624 1985.

Keywords: *Surface chemistry, *Chemisorption, *Carbon monoxide, *Potassium, Interactions, Chemical bonds, Ruthenium, Desorption, Reprints, Electron stimulated desorption.

Recent studies of CO+K on Ru(001) revealed an anomalously low CO stretching frequency of 1460/cm for low CO and K coverages. Hoffmann and de Paola proposed a side-on bound molecule with the CO molecular axis parallel to the metal surface: Weimer and Umbach suggested that CO is bound perpendicular to the surface, as on clean Ru(001), but that the CO is s(p sup 2) hybridized in the presence of K(ads). The main objectives of the present work were to search for configurational changes of adsorbed CO on K + Ru(001) and to compare these results with CO + O(ad). The authors used the ESDIAD (electron stimulated desorption ion angular distribution) method in combination with LEED (low energy electron diffraction) and TDS (thermal desorption spectroscopy).

*600,337*
**PB86-187713** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Stochastic Model for Predicting the Service Life of Photolytically Degraded Polymethyl Methacrylate Films.**
Final rept.,
J. W. Martin. 1984, 18p
Pub. in Jnl. of Applied Polymer Science 29, n3 p777-794 1984.

Keywords: *Polymethyl methacrylate, Acrylic resins, Photodegradation, Quantum effiency, Markor processes, Molecular weight, Stochastic processes, Reprints, Poisson processes.

A general stochastic model is proposed for predicting the service life of a polymeric film subjected to photodegradation. The model has two parts. One part models the arrival of successful chain scission causing photons as a function of both temperature and irradiance. The other models material degradation as a function of the number of successful chain scissions. Two indicators of degradation are used in the paper-(1) changes is the weight average molecular weight and (2) changes in the glass transition temperature. The model is partially validated against twenty-five published data sets.

*600,338*
**PB86-187762** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Dipole Threshold Laws for Single and Double Detachment from Negative Ions.**
Final rept.,
C. H. Greene, and A. R. P. Rau. Sep 85, 5p
Grants NSF-PHY82-11387, NSF-PHY81-20243
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review A 32, n3 p1352-1356 Sep 85.

Keywords: *Anions, Cross sections, Dipoles, Reprints, *Photodetachment, Hydrogen ions 1 minus, Threshold effects.

The threshold behavior of the cross section when electron detachment leaves behind a neutral atom (or molecule) with an electric dipole moment is derived through the formalism of quantum-defect theory. The cross section is a constant with a superimposed modulation with energy which has negligible amplitude for realistic situations such as the photodetachment of H(1-) accompanied by excitation. The threshold behavior for double detachment is also derived on the basis of a Coulomb-dipole description of the two electrons. It is shown that no oscillations will be observed in the cross section for this process.

*600,339*
**PB86-189073** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Planar Diffusive Motion of Alkali-Metal Intercalant Atoms in Graphite.**
Final rept.,
H. Zabel, A. Magerl, A. J. Dianoux, and J. J. Rush. 1983, 4p
Pub. in Physical Review Letters 50, n26 p2094-2097 1983.

Keywords: *Graphite, *Diffusion, Alkali metals, Neutron scattering, Reprints, *Intercalation, Quasi-elastic scattering, Structure factors.

No abstract available.

*600,340*
**PB86-189115** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Chemical Theory of Graphite-like Molecules.**
Final rept.,
S. E. Stein, and R. L. Brown. 1985, 5p
Pub. in Carbon 23, n1 p105-109 1985.

Keywords: *Graphite, *Molecular theory, Chemical reactivity, Molecular orbitals, Molecules, Reprints, Resonance radiation.

Graphite is composed of very large, highly condensed benzenoid polyaromatic molecules whose electronic properties can, in principle, be examined by conventional chemical theory. In the work, the authors present initial results of calculations on well-defined benzenoid molecules containing as many as 3300 carbon atoms. Computation times are held to practical levels using theories that require as input only counts of Kekule structures along with an efficient algorithm for counting these structures in polyaromatic molecules. These 'structure-counting' theories are particularly suited for these calculations since they have been shown to both accurately correlate a wide range of properties of polyaromatic species and yield resonance energies and reactivity indicies in good agreement with those of more sophisticated, but more time consuming, molecular orbital calculations.

*600,341*
**PB86-189149** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Millimeter Wave Spectrum of Chlorine Nitrate.**
Final rept.,
R. D. Suenram, and F. J. Lovas. 1984, 9p
Pub. in Jnl. of Molecular Spectroscopy 105, n2 p351-359 1984.

Keywords: *Microwave spectra, Millimeter waves, Rotational spectra, Molecular vibration, Excitation, Atmospheric composition, Stratosphere, Reprints, *Chlorine nitrate(ClNO3), Chlorine 35, Chlorine 37.

New measurements of the millimeter wave spectra of the (35)Cl and (37)Cl, isotopic forms of chlorine nitrate in the ground and lowest vibrational state have been made in the 80-228 GHz region. These measurements allow accurate frequency predictions of all strong transitions up to 300 GHz. A comparison of rotational line intensities with those of ClO, which has already been observed in the stratosphere, is provided. The measured and calculated frequencies of ClNO3 are available on magnetic tape.

*600,342*
**PB86-189685** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Infrared Spectra and Band Strengths of the Fundamental and First Overtone of HCl and DCl in Liquid Xenon Solutions.**
Final rept.,
J. T. Knudtson, and E. Weitz. 1985, 7p
Grant DAAG29-82-K-0125
Sponsored by Army Research Office, Arlington, VA.
Pub. in Jnl. of Chemical Physics 83, n3 p927-933, 1 Aug 85.

Keywords: *Hydrogen chloride, Deuterium compounds, Infrared spectroscopy, Liquefied gases, Cryogenics, Reprints, Liquid xenon.

The band strengths of the fundamental and first overtone of HCl and DCl have been measured in liquid xenon solution. The fundamental increases in intensity while the overtone decreases in intensity relative to the respective gas phase values. A variety of simple models are applied to the system in an effort to explain the observed effects. The possible effect of HCl-Xe complexes on the spectra is considered.

*600,343*
**PB86-189693** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Ouantum Physics Div.
**Branching Ratios for Electronically Excited Oxygen Atoms Formed in the Reaction of N(+) with O(sub 2) at 300 K.**
Final rept.,
A. O. Langford, V. M. Bierbaum, and S. R. Leone. 1986, 9p
Grant F49620-83-X-0013
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. Chemical Physics 84, n4 p2158-2166, 15 Feb 86.

Keywords: *Excitation, *Oxygen, Chemiluminescence, Electron emission, Reprints, *Ion-molecule collisions, *Oxygen atoms, *Nitrogen ions, Flowing afterglow.

Absolute branching ratios for production of O(triplet P), O(singlet D), and O(singlet S) in the reaction of N(sup +) with O2 are measured using the flowing afterglow/visible chemiluminescence technique. The O(1S) product is monitored by the O(1S)-O(1D) emission at 557.7 nm. The O(1D) product is monitored via sensitized fluorescence at 760 nm from O sub 2(sub 1) sigma (sub g)(sup +)) formed by energy transfer from O(1D) to O(sub 2)((x sup 3)(sigma(subg)(sup-)). Absolute O(1D) and O(1S) yields of 70 plus or minus 30% and less than or equal to 0.1%, respectively, of the total atomic oxygen product are inferred by comparison to the known O(1S) and O sub 2((sub 1) sigma(sub g)(sup +)) emission intensities from the reaction of Ar(triplet P) with O2. The low O(1S) yield is also obtained directly from the relative O(1S) and O sub 2((sub 1)signma(sub g)(sup +)) emission intensities from the title reaction. A qualitative reaction mechanism consistent with these observations is presented.

*600,344*
**PB86-189719** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Nascent Rotational and Vibrational Product State Distribution in the Charge Transfer Reaction of N(+) + CO yields CO(+) + N at Near Thermal Energy.**
Final rept.,
G. H. Lin, J. Maier, and S. R. Leone. 1986, 7p
Grants NSF-PHY82-00805, NSF-CHE79-11340
Sponsored by National Science Foundation, Washington, DC., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics 84, n4 p2180-2186, 15 Feb 86.

Keywords: *Carbon monoxide, Chemical analysis, Vibration, Rotation, Transport properties, Reprints, *Ion-molecule collisions, Charge exchange reactions, Nitrogen ions, Flowing afterglow.

An improved ion beam apparatus is used to measure the nascent product state distribution in the charge transfer reaction N+ + CO->CO+ + N under single-collision conditions at 0.16 eV energy. At the energy, the major vibrational channel in the CO+ products is v = 1, in contrast to the predominant formation of v = 0 at thermal energy. The relative vibrational distribution for the N+ + CO reaction is (0.40 plus or minus 0.07)sub nu = 0: (0.57 plus or minus 0.04)sub nu = 1: (0.03 plus or minus 0.01)sub nu = 2. In the v = 0 channel, the rotational distribution under single-collision conditions can be characterized by a Boltzmann distribution with a temperature of T = 410 plus or minus 40 K. In the nu = 1 channel the rotational distribution is highly excited and non-Boltzmann. The lower rotational states approximate a very high temperature of 2000K. For high rotational quantum numbers (K>23), the rotational temperature is about T = 810 plus or minus 20K. The dramatic differences in the rotational distributions are clear evidence that these two vibrational channels are formed by different reaction mechanisms, most likely a direct reaction for nu = 0, and an intimate collision for nu = 1.

*600,345*
**PB86-189727** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Ion Association and Dipolar Dumbbells: Solutions of the HNC (Hypernetted Chain) and HNC/MS (Mean Spherical) Approximations at L = sigma/2 and sigma/3 for the Sticky Electrolyte Model.**
Final rept.,
J. C. Rasaiah, and S. H. Lee. 1985, 12p
Grant NSF-CHE83-05747
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 83, n11 p5870-5881, 1 Dec 85.

Keywords: *Electralytes, Mathematical models, Reprints, Percus - Yevick equation, *Hypernetted chain approximation.

The authors extend an earlier analytic study of a sticky electrolyte model(SEM) to the case L = sigma/3, where L is the distance at which positive and negative ions bind to each other, using the hypernetted chain (HNC) approximation within the spherical core and the mean spherical approximation (MSA) outside. They also present numerical solutions to the HNC approximation alone for sigma/3 < or = L < or = sigma/2. The average number of bonded pairs is found to be essentially the same for the two approximations but the ion-ion correlation functions are very different except at high concentrations when the shielding is large. Small amounts of tetramers are also observed in the HNC correlation functions for sigma/3 less than L < or = sigma/2, and trimers are found when L = sigma/2. An expression for the excess free energy of the SEM electrolyte is derived by turning on the stickiness between oppositely charged ions. The excess energy of the system of dipolar dumbbells with charges at a distance L = sigma/3 is obtained in the MSA and the atom-atom correlation functions are compared with the HNC approximation and with recent Monte Carlo simulations. The asymptotic form of the direct correlation functions defined through the Ornstein-Zernike equation is given for dipolar dumbbells.

*600,346*
**PB86-189735** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Equilibrium Properties of Charged Hard Spheres with Adhesive Interactions between Oppositely Charged Ions.**
Final rept.,
J. C. Rasaiah, and S. H. Lee. 1985, 9p
Grant NSF-CHE83-05747
Pub. in Jnl. of Chemical Physics 83, n12 p6396-6404, 15 Dec 85.

Keywords: *Electrolytes, Chemical equilibrium, Thermodynamic properties, Adhesion, Interactions, Phase transformations, Ions, Reprints, Wiener-Hopf factorization, Percus-Yevick equation.

The equilibrium properties of charged hard spheres with adhesive interactions between oppositely charged ions are studied in the hypernetted chain/mean spherical (HNC/MS) approximation which are solved analytically. Numerical solutions to the hypernetted chain (HNC) approximation for the model are also compared with the HNC/MS approximation for a model 2-2 electrolyte in the preparative concentration range. The effect of adhesion on the low density phase transition of the primitive model electrolyte is found to be slight in contrast to the effect of charge on the phase separations at high densities of a two component mixture of hard spheres in which there is adhesion only between molecules of different species.

*600,347*
**PB86-189750** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Time-Dependent Approach to the Magnetic-Field-Induced Redistribution of Oscillator Strength in Atomic Photoabsorption.**
Final rept.,
W. P. Reinhardt. 1983, 7p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 16, n21 pL635-L641, 14 Nov 83.

Keywords: Magnetic fields, Reprints, *Photoabsorption, *Oscillator strengths.

A time dependent wave packet approach is presented as a description of the dynamics responsible for the oscillatory observed structure near the zero field ionization threshold for atomic photoabsorption in a magnetic field. The description has a simple classical interpretation which both complements and extends earlier one dimensional WKB work. Absolute positions of the oscillations, widths, and amplitude modulations are correctly accounted for. Oscillatory structure in photodetachment of negative ions in either magnetic or electric fields is predicted for appropriate polarization.

*600,348*
**PB86-189768** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Floquet-Liouville Super-Matrix Approach for Multiphoton Non-Linear Optical Processes in Intense Laser Fields.**
Final rept.,
T. S. Ho, and S. I. Chu. 1985, 6p
Sponsored by Department of Energy, Washington, DC., and American Chemical Society, Washington, DC.
Pub. in Chemical Physics Letters 122, n4 p327-332, 13 Dec 85.

Keywords: Eigenvalues, Reprints, *Multi-photon processes, Resonance fluorescence, Floquet function, Liouville equations, Nonlinear optics, Laser radiation.

A practical non-perturbative approach is presented for the treatment of multiphoton non-linear optical processes in intense monochromatic or polychromatic field. By extending the many-mode Floquet theory recently developed by the authors, the time-dependent Liouville equation for the density matrix of atoms or molecules undergoing radiative and/or collisional relaxations can be transformed into an equivalent time-independent Floquet-Liouville super-matrix eigenvalue problem. The method is illustrated by a study of the multiphoton resonance fluorescence spectra of two-level systems.

*600,349*
**PB86-190642** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.

**Multivacancy Effects in the X-ray Spectra of CH3Cl.**
Final rept.,
R. C. C. Perera, J. Barth, R. E. LaVilla, R. D. Deslattes, and A. Henins. 1985, 6p
Grant DE-AC03-76SF00098
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A: General Physics 32, n3 p1489-1494 Sep 85.

Keywords: *X ray spectra, *Chloromethanes, Absorption, X ray spectroscopy, Emission spectra, Excitation, Reprints, Methyl chloride.

A high-efficiency x-ray spectrometer has been constructed with use of a curved crystal and a position-sensitive detector mounted along a Rowland circle. Results obtained for the ClK absorption and fluorescent K beta emission of molecular CH3Cl show previously unobtainable details. The gas target is excited by primary radiation from a demountable conventional x-ray tube. The use of different anode materials and the insertion of filters between x-ray source and target allow some variation of the primary excitation energy. By monitoring emission spectra for different primary excitation energies, we are able to attribute the newly observed absorption features to multivacancy excitations. Such modulations in the suprathreshold absorption cross section would complicate the extraction of structural information in an extended x-ray-absorption fine-structure (EXAFS) analysis.

*600,350*
**PB86-190675** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Hydrogen Bond Energies of the HF and HCl Dimers from Absolute Infrared Intensities.**
Final rept.,
A. S. Pine, and B. J. Howard. 1986, 7p
Pub. in Jnl. of Chemical Physics 84, n2 p590-596, 15 Jan 86.

Keywords: *Dissociation energy, *Hydrogen bonds, *Hydrogen chloride, *Hydrogen fluoride, Infrared radiation, Reprints, *Dimers, Tunable lasers.

The dissociation energies of the hydrogen-bonded complexes, (HF)2 and (HCl)2, have been obtained from high-resolution measurements of absolute infrared line strengths at a single temperature and pressure under the assumption of minimally perturbed local-mode behavior of the outer hydrogen stretch. The zero-point dissociation energies for the HF and HCl dimers are D sub zero = 1038( +43, -34) and 431(plus or minus 22)/cm-1, respectively. Estimates of the zero-point energies of the low frequency intermolecular vibrations enable us to obtain the well depths and equilibrium dissociation energies for comparison to ab initio calculations and empirical models.

*600,351*
**PB86-191418** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Non-Adiabatic Effects in Elementary Surface Reactions: State-to-State Molecular Beam Experiments as a Probe.**
Final rept.,
J. W. Gadzuk. 1984, 16p
Grant NSF-PHY77-27084
Sponsored by National Science Foundation, Washington, DC.
Pub. in Many-Body Phenomena at Surface, p517-532 1984.

Keywords: *Surface chemistry, *Surfaces, Chemical reactions, Diatomic molecules, Excitation, Surface reactions, Surface scattering, Vibrational energy levels.

A theory of elementary chemical reactions at solid surfaces is described in terms of surface induced diabatic transitions between 'reactant' and 'product' potential curves. It is then shown how the internal vibrational state distribution of a diatomic molecule scattered from a surface could provide unique dynamical information required as input to the diabatic transition theory.

*600,352*
**PB86-191434** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

**Interaction of Physisorbed Species with Chemisorbed Species as Studied by Infrared Spectroscopy.**
Final rept.,
J. T. Yates, and G. L. Haller. 1984, 5p
Pub. in Jnl. of Physical Chemistry 88, n20 p4660-4664 1984.

Keywords: *Chemisorption, *Carbon monoxide, Surface chemistry, Adsorption, Rhodium, Aluminum oxide, Reprints.

Infrared spectroscopy has been used to study the physical adsorption of CO onto a Rh/Al2O3 surface. In addition to absorption bands related to monolayer and multilayer physisorbed CO species, an interaction between the physisorbed species and chemisorbed CO has been observed causing a decrease of the chemisorbed CO wavenumber. Similar effects between physisorbed Xe and chemisorbed N2 on Rh surfaces have also been observed, suggesting that the effect is a general one. Correlation of these measurements with measurements of CO trapped in CO matrices suggests that inductive and dispersive effects are the main factors responsible for the negative shift in chemisorbed species wavenumber. It has been found that physisorbed CO preferentially adsorbs in the vicinity of ionic sites.

*600,353*
**PB86-191442** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Single-Pulse Shock-Tube Studies on the Decomposition of 1,2-Dibromoperfluoroethane and Allyl Bormide.**
Final rept.,
W. Tsang. 1984, 6p
Pub. in Jnl. of Physical Chemistry 88, n13 p2812-2817 1984.

Keywords: *Decomposition, Chemical reactions, Cyclopentane, Chemical radicals, Reprints, *Bromide/allyl, *Ethane/dibromo-perfluoro, *Chemical reaction kinetics, Collision rates, Shock tubes.

1,2-Dibromoperfluoroethane and allyl bromide have been decomposed in comparative rate single pulse shock tube experiments. Cyclopentane is used as a radical trap and as a source of the ethylene which serves as a direct measure of the number of radicals generated in the system. Under the reaction conditions both decomposition processes (1) BrCF2CF2Br -> Br + C2F4Br (radical), and (2) Allyl Br -> allyl + Br (radical) are in the beginning of the fall-off region, k/k(sub infinity) greater than or approx. equal to 0.7 RRKM calculations yield the following high pressure rate expressions.

*600,354*
**PB86-192150** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Kinetics and Mechanisms of Hydroxyl Radical-Induced Crosslinks between Phenylalanine Peptides.**
Final rept.,
M. G. Simic, E. Gajewski, and M. Dizdaroglu. 1984, 8p
Pub. in Radiation Physics and Chemistry 24, n5-6 p465-473 1984.

Keywords: *Peptides, *Phenylalanine, Chemical reactions, Gas chromatography, Mass spectroscopy, Reprints, *Chemical reaction kinetics, *Hydroxyl radicals, Dimerization, Pulse radiolysis.

Reactions of OH radicals with phenylalanine (Phe) and its homopeptides, i e. L-Phe-L-Phe and L-Phe-L-Phe-L-Phe, in N2O-saturated aqueous solutions were investigated by pulse radiolysis, high-performance liquid chromatography and mass spectrometry. For identification of radiation-induced products, samples of irradiated Phe and HCl-hydrolyzates of its irradiated homopeptides were trimethylsilylated and analyzed by capillary gas chromatography-mass spectrometry. Mass spectra of the trimethylsilylated products revealed the formation of o-, m- and p-tyrosines and biphenyl type dimers. G-Values of these products were also determined by gas chromatography. Mechanisms of product formation were discussed in detail.

*600,355*
**PB86-192457** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.

**Vibrations of Crystallographic Defects Associated with a Single Chain in Polyethylene.**
Final rept.,
D. H. Reneker, and J. Mazur. 1984, 13p
Pub. in Polymer 25, n11 p1549-1561 1984.

Keywords: *Polyethylene, *Crystal defects, *Molecular vibration, Crystallography, Dispersion, Dislocations(Materials), Reprints.

The vibrational behavior of crystallographic defects associated with a single chain were investigated for a dispiration, disclination, and dislocation in polyethylene. An approximate longitudinal modulus for the defects was determined by using conformational calculations to estimate the energy changes associated with changes in length of a defect. The modulus, combined with the mass per unit length of the defect, was used to estimate the lowest longitudinal frequency of the defect, which was found to be around 100/cm for all the defects considered. Normal mode vibrational calculations for oligomers containing defects showed that the predicted lowest longitudinal modes could be identified by examination of the displacements associated with modes occurring in the estimated frequency range. It was shown that the defects could be considered as localized oscillators embedded in the crystal and coupled to the vibrational modes of the crystal. The presence of defects provides special mechanisms for coupling light waves and lattice vibrations in the crystal which may affect the Raman spectrum.

*600,356*
**PB86-192481** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
**State-to-State Differential and Integral Cross Sections for Vibrational-Rotational Excitation and Elastic Scattering of Electrons by Nitrogen at 5-50 eV: Calculations using Extended-Basis-Set Hartree-Fock Wave Functions.**
Final rept.,
J. R. Rumble, D. G. Truhlar, and M. A. Morrison. 1983, 13p
Sponsored by National Center for Atmospheric Research, Boulder, CO., and National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 79, n4 p1846-1858 1983.

Keywords: *Nitrogen, *Electron scattering, Differential cross sections, Elastic scattering, Excitation, Reprints, *Electron-atom collisions.

The authors have calculated differential, integral, and momentum-transfer cross sections for vibrational-rotational excitation as well as pure rotational excitation, pure vibrational excitation, and elastic scattering for electron collisions with N2 at 5-50 eV impact energy. The interaction potential has three terms: static and local exchange potentials calculated from extended-basis-set Hartree-Fock wavefunctions as functions of internuclear distance and a semiempirical polarization potential. The results are compared to previous calculations and to experiment.

*600,357*
**PB86-192523** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Resonance Vibrational Excitation in Electron-Energy-Loss Spectroscopy of Adsorbed Molecules.**
Final rept.,
J. W. Gadzuk. 1985, 3p
Pub. in Physical Review B: Solid State 31, n10 p6789-6791, 15 May 85.

Keywords: *Adsorption, Excitation, Surfaces, Interactions, Molecular vibration, Reprints, *Energy-loss spectroscopy, Electron-molecule collisions.

A mechanism is suggested which could lead to enhanced excitation of the low-frequency vibrational modes associated with the bond between a solid surface and a molecule adsorbed upon it or of hindered rotational modes with displacement components normal to the surface, as observed in electron-energy-loss spectroscopy. If the incident electron becomes trapped in a negative-molecular-ion shape resonance, manifesting itself in significant intramolecular overtone excitation, the molecule-surface potential-energy curve is augmented by the image potential of the negative ion. This allows displacement of the molecule from its equilibrium neutral position which in turn appears as

vibrational excitation of adsorbate-substrate relative motions, upon return to the neutral curve. A simple theory for the effect is presented and numerical estimates of its magnitude are given.

*600,358*
**PB86-192986** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Role of Standards in Secondary Ion Mass Spectrometry.**
Final rept.,
D. E. Newbury, and D. Simons. 1984, 6p
Pub. in Springer Ser. Chem. Phys. 36, p101-106 1984.

Keywords: *Mass spectroscopy, Standards, Ions, Reprints, *Secondary ion mass spectroscopy, Ion microprobe analysis, Ion microscopes, Sensitivity analysis.

The existence of strong matrix and instrumental effects in secondary ion mass spectrometry procludes the use of theoretical models for accurate quantitative elemental analysis. Standards must be employed to reduce problems associated with instrumental effects and matrix effects. By means of relative elemental sensitivity factors based on glass standards, analysis with errors of 20% relative or less is feasible, even for trace elements.

*600,359*
**PB86-193018** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Diode Laser Spectra of Cis-Nitrous Acid Near 850/cm and Trans-Nitrous Acid Near 1700/cm.**
Final rept.,
A. G. Maki, and R. L. Sams. 1983, 7p
Pub. in Jnl. of Molecular Structure 100, p215-221 1983.

Keywords: *Nitrous acid, *Molecular isomerism, Infrared spectroscopy, Absorption spectra, Frequencies, Reprints, High resolution.

Tunable diode laser spectra have been measured for the nu sub 4 band of cis-HONO near 850/cm and the nu sub 2 band of trans-HONO near 1700/cm. The nu sub 4 band is completely unperturbed and 355 well resolved transitions have been fit with a standard deviation of 0.0007/cm. The nu sub 2 band appears to have some small perturbations, but about 190 transitions have been fit with a standard deviation of 0.0027/cm. Rotational and centrifugal distortion constants are given for both bands.

*600,360*
**PB86-193026** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**ns Rydberg Series of 1,3-Trans-Butadiene Observed Using Multiphoton Ionization.**
Final rept.,
W. G. Mallard, J. H. Miller, and K. C. Smyth. 1983, 6p
Pub. in Jnl. of Chemical Physics 79, n12 p5900-5905 1983.

Keywords: *Butadienes, Reprints, *Multiphoton ionization, *Rydberg series, Diffusion flames, Core sampling.

The ns Rydberg series of 1,3-trans-butadiene has been observed in a diffusion flame environment using two-photon resonant multiphoton ionization in the 330-269 nm wavelength region. An analysis of the energies for the N=4 to N=10 states yields a series limit of 73172 + or - 22/cm and a quantum defect of 0.91 + or - 0.04. The ns series limit has been averaged with the limits of three other Rydberg series to give an ionization potential of 73154 + or - 30/cm. The 3s and 4s states show substantial effects of mixing with the core orbitals.

*600,361*
**PB86-193034** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Real-Time Mass-Spectrometric Study of the Chemistry Initiated by Infrared-Laser Photolysis: CF2Cl2.**
Final rept.,
R. I. Martinez, and J. T. Herron. 1983, 6p
Pub. in Chemical Physics Letters 98, n2 p184-189 1983.

Keywords: *Reaction kinetics, Chemical analysis, Free radicals, Photolysis, Mass spectroscopy, Infrared spectroscopy, Reprints, *Methane/dichloro-difluoro, *Ethylene/tetrafluoro, Real time measurements.

The infrared-laser photolysis/mass-spectrometric (ILP/MS) technique was used to monitor directly in real time the free-radical and stable reactants and products present in the reactive system initiated by the multiphoton-induced dissociation of CF2Cl2. It was found that, contrary to conclusions based on final-products analyses, the C2F4 observed as a final product in the system is not formed solely through the recombination of:CF2 radicals, but rather C2F4 is produced in a complex series of secondary reactions.

*600,362*
**PB86-193117** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Heterodyne Frequency Measurements on N2O between 1257 and 1340/cm.**
Final rept.,
J. S. Wells, A. Hinz, and A. G. Maki. 1985, 13p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Molecular Spectroscopy 114, p84-96 1985.

Keywords: *Nitrous oxide, Absorption spectra, Frequency measurement, Frequency standards, Demodulation, Reprints, Laser applications, Tunable lasers, Infrared radiation.

Frequency measurements are given for the (00 sup 0)1 - (00 sup 0)0 and (01 sup 1)1 - (01 sup 1)0 bands of N2O from 1257 to 1340/cm. The measurements utilize heterodyne techniques by measuring small frequency differences between a tunable diode laser locked to the center of an N2O absorption line and harmonic combinations of frequencies of radiation from two CO2 Lamb-dip-stabilized lasers. The measurements are facilitated by the use of the CO laser as a transfer laser whose frequency is also measured. These measurements have been combined with other data to provide new band constants and frequency calibration tables for several band systems of N2O in the following regions; 1215 to 1340, 1816 to 1930, and 2135 to 2268/cm. A correction factor is also provided for existing calibration tables near 590/cm.

*600,363*
**PB86-193141** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Electronic Structure and Spectra of UO(1+).**
Final rept.,
M. Krauss, and W. J. Stevens. 1983, 5p
Pub. in Chemical Physics Letters 99, n5-6 p417-421, 19 Aug 83.

Keywords: *Uranium oxides, Visible spectrum, Infrared spectra, Reprints, *Electronic structure, Relativistic effects.

Relativistic effective potentials are used to calculate the electronic structure and spectroscopic properties of UO(1+). The lowest energy states are very ionic and the molecular orbitals substantially localized so that the molecule is described by the ionic fragments, U(+3)(f sup 3, 4l) and O(-2)(singlet 1). All of the quartet states from Sigma (sup-) to I, that arise from the coupling of these ionic fragments, are perturbatively mixed using an effective operator for the spin-orbit. The Re and Omega sub e of the ground Omega = 9/2 state have been determined to be 3.48 bohr and 925/cm. The vibrational and electronic states are interleaved with the lowest excited state, Omega = 7/2, at 1315/cm. The excitation energies of the excited states of UO(1+) were calculated using a restricted valence configuration interaction. Strong radiative transitions are predicted in the red part of the visible. These transitions are predominately atomic-like f to d.

*600,364*
**PB86-193190** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Multiple Ionization and the Charged State Evolution of Ions Exposed to Electron Impact.**
Final rept.,
A. Mueller. 1986, 5p
Pub. in Physics Letters 113A, n8 p415-419, 13 Jan 86.

Keywords: *Gas ionization, Electric charge, Reprints, *Electron-atom collisions, EV range 100-1000.

Charge state abundances of atoms exposed to an electron flux for a time t are calculated from experimental cross sections by considering either electron impact single ionization only or by including multiple ionization. When multiple ionization is neglected (Xe sup qt) ion abundances (q=0,1,...,6) for an electron energy of 700 eV are off by a factor of up to 2 both in peak size and in time necessary to reach the peak value.

*600,365*
**PB86-193299** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Neutron Spectroscopic Studies of the Adsorption and Decomposition of C2H2 and C2H4 on Raney Nickel.**
Final rept.,
R. D. Kelley, R. R. Cavanagh, J. J. Rush, and T. E. Madey. 1985, 19p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Surface Science 155, p480-498 1985.

Keywords: *Chemisorption, *Catalysts, *Nickel, Surface chemistry, Adsorption, Ethylene, Acetylene, Decomposition, Neutron scattering, Reprints.

Incoherent neutron inelastic scattering has been applied to the study of the chemisorption of C2H2 and C2H4 on Raney nickel (a high surface area nickel powder) as a function of temperature. Surface vibrational spectra of the adsorbed layer obtained through neutron scattering demonstrate that at 150 K C2H2 adsorbs molecularly on the nickel surface. Ethylene, however, is more reactive. Even at 120 K there is some C2H4 decomposition. In addition, perdeuteroethylene coadsorbed with atomic hydrogen undergoes isotopic exchange at 120 K. As the temperature is raised to 275 K both hydrocarbons decompose. The vibrational spectra of the molecularly adsorbed species are similar to those observed on flat Ni(111) single crystal surfaces with EELS. However, the decomposition process at higher temperature is not simply related to results reported on either flat or stepped Ni(111) surfaces. The authors conclude that the dominant influence of steps (or other defect structures) on high surface area nickel powders is to lower the activation energy for dissociation.

*600,366*
**PB86-193323** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Structure of the Surface Hydration Shell of Bromide on Ag(110).**
Final rept.,
K. Bange, T. E. Madey, and J. K. Sass. 1985, 7p
Sponsored by Department of Energy, Washington, DC., and Deutsche Forschungsgemeinschaft, Bad Godesberg (Germany, F.R.).
Pub. in Surface Science 162, p252-258 1985.

Keywords: *Surface chemistry, *Sorption, *Bromine, *Silver, Desorption, Adsorption, Water, Electrochemistry, Reprints, *Electron stimulated desorption ion angular distribution.

The interaction of water and bromine on Ag(110) has been studied in the temperature range 80-300 K, using ESDIAD (electron stimulated desorption ion angular distribution), LEED (low energy electron diffraction) and TDS (thermal desorption spectroscopy). Compared to the clean surface, water adjacent to surface bromide was characterized by a higher binding energy and pronounced orientational order. The mixed adlayers resulting from the surface hydration of bromide exhibited long-range order. The surface hydration number (n sub H2O/n sub Br) was two for Theta sub Br < or approx = 0.25 and decreased to a few tenths at the bromine saturation coverage Theta sub Br approx. equal 0.75. Comparison is made to the results of a recent similar study on Cu(110) and electrochemical aspects are briefly considered.

*600,367*
**PB86-193331** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Application of Decelerated Bare Nuclei to Precision Spectroscopy of One-Electron Ions.**
Final rept.,
R. D. Deslattes, R. Schuch, and E. Justiniano. Sep 85, 3p
Pub. in Physical Review A: General Physics 32, n3 p1911-1913 Sep 85.

Keywords: *Ions, X ray spectra, Reprints, *Chlorine ions, Lamb shift.

Bare Cl nuclei were decelerated and then allowed to capture a single electron in a He-gas target. By the method pure hydrogenlike Cl ions were prepared in an excited state from which the 2p-1s transition wavelength could be accurately (about 0.00001) measured without distortion by spectator electrons. After Doppler correction utilizing measurements at four different ion velocities (vc about = 0.038-0.067), fine-structure splitting and 1s Lamb-shift values were determined within 15% error bars, which, while far from the potential possible limits of our method, are in agreement with theoretical results.

*600,368*
**PB86-193349** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Fundamental and Incidental Limits on the Spectroscopy of Single Electron Ions.**
Final rept.,
R. D. Deslattes. 1985, 5p
Pub. in Nuclear Instruments and Methods in Physics Research B9, p668-672 1985.

Keywords: *Spectroscopy, *Ions, Reprints, Quantum electrodynamics, Lamb shift.

Precision measurements of spectra from one-electron ions are principally focused on tests of QED corrections to the energy levels implied by the Dirac equation. Even though spectroscopic tests in atomic hydrogen itself and determination of the anomalous moment of the electron have reached impressive levels of refinement and demonstrate equally impressive consistency between experiment and theory, exploration of the Z-dependence of such comparisons remains of interest. Fundamentally, such 'Lamb-shift' experiments are characterized by and are limited by some 'Q-value' determined by the magnitude of the QED shift, S, in relation to a line-width parameter, gamma. Such Q-values are rather small for the traditional delta n=0 experiments, regardless of Z. Substantial improvement in the regard is available if one studies deltan=1 transitions, but in these cases there is a substantial, though largely incidental, penalty in loss of 'leverage' in the measurement. Additionally, and also incidentally, the earliest example of such deltan =1 experiments have suffered from various combinations of Doppler troubles and spectator electron perturbations. Only in one very recent effort has it been possible to bring both of these problems under simultaneous control thereby inviting consideration of a still more refined level at which fundamental limitations again appear dominant.

*600,369*
**PB86-193588** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Time-Resolved Measurements of OH(v=1) Vibrational Relaxation on SiO2 Surfaces: Isotope and Temperature Dependence.**
Final rept.,
M. P. Casassa, E. J. Heilweil, J. C. Stephenson, and R. R. Cavanagh. 1986, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics 84, n4 p2361-2364, 15 Feb 86.

Keywords: *Surface chemistry, *Surfaces, *Silicon dioxide, Chemisorption, Molecular relaxation, Energy transfer, Reprints, Temperature dependence, Time dependence, Multiphonon processes, Picosecond pulses.

Picosecond infrared spectroscopy was used to measure the vibrational energy relaxation time T1 of OH(Nu=1) and OD(Nu=1) groups chemisorbed on silica surfaces over the temperature range 100 less than or equal to T less than or equal to 800K. The observed T1 times and their temperature dependencies are discussed in terms of a multiphonon relaxation mechanism. Limiting low temperature lifetimes are T1=220 plus or minus 20 ps (1 sigma) for OH(Nu=1) and T1=149 plus or minus 10 ps for OD(Nu=1).

*600,370*
**PB86-193620** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Symmetry beyond Point Groups in Molecular Spectroscopy.**
Final rept.,
J. T. Hougen. 1986, 7p
Pub. in Jnl. of Physical Chemistry 90, n4 p562-568 1986.

Keywords: *Molecular spectroscopy, Group theory, Reprints, Point groups.

An attempt is made to distill from the published literature a summary of some new uses of group theory in high resolution gas-phase spectroscopic studies of molecules with large amplitude and/or tunneling motions, paying particular attention to questions like the following: (i) When is a point group sufficient, and when is it not. (ii) What kind of information is easy, and what kind is difficult to extract from a permutation-inversion group treatment. (iii) What seem to be the advantages and disadvantages of various extended groups of the permutation-inversion group. While most spectroscopists would agree that a general group theoretical approach, suitable for application without modification to the majority of floppy molecules, has not yet been synthesized from the particular cases studied in the literature, some feeling for one direction of progress in the field can be obtained from the several examples presented.

*600,371*
**PB86-193729** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Optical and Electrical Analysis of Blue Polymethyl Methacrylate for High-Dose Dosimetry.**
Final rept.,
N. S. I. Rageh, N. B. El-Assy, M. Ashry, and W. L. McLaughlin. 1986, 5p
Pub. in Radiation Physics and Chemistry 27, n2 p127-131 1986.

Keywords: *Dosimetry, *Plastics, Conductivity, Reprints, Polymethyl methacrylate.

The response to gamma radiation of polymethyl methacrylate ('blue PMMA') containing a blue dye was investigated, with the aim of providing a high-dose dosimeter based on either spectrophotometry or electrical-conductivity measurements. It is found that the 3-mm thick pieces of blue PMMA can be used for dosimetry in a range of absorbed doses from about 5-50 kGy, for which the changes in optical transmission density (absorbance) at different wavelengths in the visible region (402, 596, 612, and 643 nm) are linear functions of dose. Results also show that irradiation of thin 0.1 mm films of blue PMMA produces two components of radiation-induced conductivity: a transient component which can be used to determine the absorbed dose rate and a steady-state component which registers the total absorbed dose in the range 20-80 kGy as based on a suitable calibration. The effects of post-irradiation storage time, day light, and storage temperature on the radiation-induced visible spectrum were investigated. The storage-temperature effect on post-irradiation conductivity measurement was also evaluated.

*600,372*
**PB86-193745** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Network Structure of Epoxies: 2. A Neutron Scattering Study.**
Final rept.,
W. Wu, and B. J. Bauer. 1986, 12p
See also PB85-229912.
Pub. in Polymer 27, p169-180 1986.

Keywords: *Epoxy resins, *Molecular structure, *Neutron scattering, *Elastic scattering, Molecular weight, X rays, Thermosets, Reprints.

Neutron scattering measurements were performed on epoxies to elucidate the molecular network structure of these commonly used thermosets. A partially deuterated diglycidyl ether of bisphenol A (DGEBA) was cured with di- and triamines based on poly(propylene oxide) chains. Pronounced neutron scattering peaks were observed on all three epoxies studied, while X-ray scattering yielded scattering typical of most amorphous materials. The neutron scattering results can be explained successfully using equations that have been derived using a result from a random phase approximation based on an ideal network. Neutron measurements were also conducted on epoxies that had been swollen in acetone. The swollen sample results, along with those from the bulk specimens, provide a unique approach to the network homogeneity problem in epoxies.

*600,373*
**PB86-193760** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Neutron Scattering Study of Zeolite Rho.**
Final rept.,
M. J. Wax, R. R. Cavanagh, J. J. Rush, G. D. Stucky, and L. Abrams. 1986, 3p
Pub. in Jnl. of Physical Chemistry 90, n4 p532-534 1986.

Keywords: *Ion exchange resins, Neutron scattering, Chemical bonds, Reprints, *Zeolite rho, Molecular sieves, Faujasite.

Incoherent inelastic neutron scattering has been used to examine the bonding of framework hydrogen to the faujasite zeolite Rho. Vibrational spectra obtained from 160 to 1600/cm are consistent with the existence of planar, symmetric AlO(H)Si units in the acid form of Rho at room temperature. As the zeolite undergoes a slight change in structure on heating, an accompanying transfer of hydrogen atoms occurs to some new bonding site of unknown nature, which is characterized by an unusually large-amplitude, low-energy vibration. Quasi-elastic neutron scattering data have allowed an upper limit to be set for the diffusion coefficient of hydrogen on the framework of partially dehydroxylated Rho, consistent with diffusion measurements by macroscopic methods.

*600,374*
**PB86-193778** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Multiphoton Dynamics and Resonance Lineshapes in Three-Level Systems: Many-Mode Floquet Treatment.**
Final rept.,
K. Wang, T. S. Ho, and S. I. Chu. 1985, 18p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, p4539-4556 1985.

Keywords: Absorption, Perturbation, Excitation, Reprints, *Multi-photon processes, *Resonance absorption, Floquet theory.

The authors present an exact treatment of two- and multiquantum transitions in three-level systems driven by two intense linearly polarized monochromatic fields based on the semiclassical many-mode Floquet theory developed recently. Further they extend the almost degenerate perturbation theory of Salwen to the two-mode Floquet Hamiltonian and obtain approximate analytical formulae for multiphoton transition probabilities, resonance bichromatic shifts and widths, and absorption lineshapes, beyond the conventional rotating-wave approximation (RWA). Detailed comparison of the analytical, the RWA, and the exact results is given. Several novel features of multiphoton lineshape characteristics are pointed out.

*600,375*
**PB86-193794** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**NBS/NRC (National Bureau of Standards/National Research Council) Steam Tables.**
Final rept.,
L. Haar, J. S. Gallagher, and G. S. Kell. 1984, 400p
Pub. in 400 pages from Hemisphere Publication Corporation, Washington, DC., 1983.

Keywords: *Water, *Steam, Thermodynamic properties, Transport properties, Surface tension, Tables(Data), Reprints, *Calibration standards.

Thermodynamic properties values for water and steam based on a new formulation derived by the authors are included at closely spaced intervals, for the range 0 < or - t < or - 2000 C and 0 < or - P < or - 30,000 bar. The formulation has been provisionally accepted (September of 1982) as the international standard for scientific and general use by the International Association for the Properties of Steam (IAPS). Also provided are IAPS approved values for the transport and other thermophysical properties, all of which have been made consistant with the thermodynamic formulation. In addition to tables and figures the book includes a discussion of the derivation and the accuracy for thermody-

namic formulation, and lists the equations approved by IAPS for the transport and the thermophysical properties.

*600,376*

**PB86-193869** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Field Effects on the Rydberg Product-State Distribution from Dielectronic Recombination.**
Final rept.,
A. Mueller, D. S. Belic, B. D. DePaola, N. Djuric, and G. H. Dunn. 1986, 4p
Contract DOE-EA-77-A-01-6010
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Physical Review Letters 56, n2 p127-130, 13 Jan 86.

Keywords: Reprints, *Magnesium ions, *Electron-ion collisions, Dielectronic recombination.

The effects of state mixing by extrinsic fields in the collision region have been investigated for the dielectronic recombination process Mg + (3s) + e -> Mg(3p,nl) -> Mg(3s,nl) + h nu. By field ionization of the Rydberg atoms produced, cross sections sigma(N sub f) have been measured. The observed large changes of sigma(N sub f) with alteration of the extrinsic field provide the first incontrovertible experimental evidence that dielectronic recombination can be changed by external fields.

*600,377*

**PB86-193877** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Raman Spectroscopy of Gases with a Fourier Transform Spectrometer: The Spectrum of D2.**
Final rept.,
D. E. Jennings, A. Weber, and J. W. Brault. 1986, 7p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Applied Optics 25, n2 p284-290, 15 Jan 86.

Keywords: *Ramon spectroscopy, *Deuterium, Hydrogen, Reprints, Fourier transform spectroscopy.

A high-resolution Fourier transform spectrometer (FTS) has been used to record spontaneous incoherent laser Raman spectra of gases. The resolution, sensitivity, calibration accuracy, and spectral coverage achieved in these spectra demonstrate the viability of the FTS for Raman spectroscopy. Measurements from a spectrum of D2 containing both v=0-0 and v=1-0 transitions were fitted to the Dunham expansion of the vibration-rotation energy levels. The coefficients are given.

*600,378*

**PB86-194974** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Studies of Thin-Films in Binary Fluid Mixtures Using Ellipsometry.**
Final rept.,
J. W. Schmidt, and M. R. Moldover. 1983, 1p
Pub. in Annals of the New York Academy of Sciences 404, p350 May 83.

Keywords: *Thin films, *Mixtures, Binary systems(Materials), Surfaces, Reprints, *Cyclohexane/methyl, *Cyclohexane/methyl-perfluoro, *Ellipsometry.

In certain binary solutions, the lower of the two liquid phases forms a layer that intrudes between the upper liquid phase and the vapor. The authors used ellipsometry to measure the intruding layer's thickness--it was between 0.7 micrometer and 4 micrometers in a system consisting of C7F14 (perfluoromethycyclohexane) and C7H14 (methycyclohexane). The thickness varies approximately as L sup -1/3, where L is the height spanned by the upper liquid phase. The behavior was predicted by de Gennes, who used the idea that the long-ranged part of the intermolecular potential governs the layer's thickness. Deviations from L sup -1/3 behavior occur near consolute points.

*600,379*

**PB86-194982** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Reaction of Oxygen and Aluminum on Rh(111).**
Final rept.,
S. Semancik. 1984, 2p
Pub. in Jnl. of Vacuum Science and Technology A-Vacuum Surfaces and Films 2, n2 p886-887 1984.

Keywords: *Aluminum, *Oxygen, Surface chemistry, Adsorption, *Aluminum oxide, Rhodium, Chemical reactions, Reprints, Low energy electron diffraction, Auger electron spectroscopy.

The initial stages of aluminum oxide formation on rhodium have been studied by absorbing oxygen and aluminum on a Rh(111) surface. Low energy electron diffraction and Auger spectroscopy were used to characterize, as a function of temperature and coverage, both individual overlayers of aluminum and oxygen on Rh, and the interaction between these species during coadsorption experiments.

*600,380*

**PB86-194990** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Study of Miscibility and Critical Phenomena of Deuterated Polystyrene and Hydrogenated Poly(vinyl methyl ether) by Small-Angle Neutron Scattering.**
Final rept.,
M. Shibayama, H. Yang, R. Stein, and C. C. Han. 1985, 9p
Pub. in Macromolecules 18, n11 p2179-2187 1985.

Keywords: *Solubility, *Polystyrene, *Polyrinyl methyl ether, Polymers, Vinyl ether resins, Length, Neutron scattering, Reprints, Small angle scattering.

Miscibility and critical phenomena were studied on the polymer system of deuterated polystyrene and hydrogenated poly(vinyl methyl ether) by the small-angle neutron scattering technique. The phase diagram was constructed with 'light' and 'neutron' cloud points as well as spinodal points. It shows a well-known behavior of a lower critical solution temperature. The agreement between the 'light' and 'neutron' cloud points is fairly good for all compositions. The correlation length, the statistical segment length, and the Flory-Huggins Chi-parameter were obtained as functions of temperature and composition by employing de Gennes' scattering equation for polymer blends. The Chi-parameter showed not only a temperature dependence but also a composition dependence. Comparison of the Chi-parameter with the lattice fluid theory shows that the composition dependence of Chi results from the lattice fluid nature of the system, i.e., the compressibility and the thermal expansion of the system.

*600,381*

**PB86-195187** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Desorption of Ions from Surfaces: Mechanisms of Photon Stimulated Desorption.**
Final rept.,
R. Stockbauer, and T. E. Madey. 1984, 8p
Pub. in Ann. Isr. Phys. Soc. 6, p483-490 1984.

Keywords: *Desorption, *Surfaces, Chemisorption, Synchrotron radiation, Reprints, *Photon stimulated desorption.

A review is given of the mechanisms of Photon Stimulated Desorption (PSD) from ionic, covalent and van der Waals bonded surfaces. An interatomic Auger decay process describes desorption from ionically bonded, maximal valency compounds. The mechanism for ion desorption from covalently bonded systems is not as well understood but is thought to involve relatively long-lived two hole states similar to doubly charged ionic states in the gas phase. Ion desorption from thick molecular films presents a challenge to theory since heavy fragments (CxHy) desorb from some (cyclohexane) and not from others (water, methanol). It is possible that hydrogen bonding or proton transfer could play a significant role in suppressing heavy fragments from the water or methanol surface.

*600,382*

**PB86-195195** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Electron Excitation of Na(3S) and Na(3P) Atoms to the Na(3D) State.**
Final rept.,
B. Stumpf, and A. Gallagher. Dec 85, 10p
Contract ARO-8-82, Grant NSF-PHY82-00805
Sponsored by Army Research Office, Research Triangle Park, NC., and National Science Foundation, Washington, DC.
Pub. in Physical Review A 32, n6 p3344-3353 Dec 85.

Keywords: *Sodium, Atomic energy levels, Excitation, Reprints, *Electron-atom collisions.

The cross sections for electron-impact excitation of Na(3S) and Na(3P) atoms to the 3D state have been measured from threshold to 1000 eV, with about 0.3 eV resolution. The 3P-state atoms are produced in the m(l)=1, m(s)=1/2 level by optical excitation, and 3D->3P fluorescence is detected at 90 degrees to the quantization axis. The resulting polarization anisotropies are considered, and included along with cascade effects in the high-energy normalizations to the Born approximation. The 3S->3D and 3P->3D excitation cross sections both rise very abruptly at threshold, and are indistinguishable from a step function with our energy resolution.

*600,383*

**PB86-195492** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Comment on 'Anomalies in Chemical Equilibrium near Critical Points'.**
Final rept.,
G. Morrison, I. Procaccia, and M. Gitterman. Jul 84, 4p
Pub. in Physical Review A 30, n1 p644-647 Jul 84.

Keywords: *Critical point, Scattering, Turbidity, Reprints, *Equilibrium constant.

An analysis of measurements purporting to show the effect of a critical point on the extent of a chemical reaction indicates that the measured phenomenon can be accounted for by turbidity at the critical point.

*600,384*

**PB86-195518** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Photodetachment Threshold of CN (1-) by Laser Optogalvanic Spectroscopy.**
Final rept.,
R. Klein, R. P. McGinnis, and S. R. Leone. 1983, 4p
Grants NSF-CHE79-11340, NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Chemical Physics Letters 100, n6 p475-478, 30 Sep 83.

Keywords: *Cyanides, Anions, Reprints, Laser spectroscopy, Optogalvannic effect, *Photodetachment.

Laser optogalvanic spectroscopy is used for the first time to obtain the photodetachment threshold for a molecular negative ion, CN(1-). The electron affinity for CN is determined to be 3.821 + or - 0.004 eV.

*600,385*

**PB86-195526** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Enskog Theory for Multicomponent Mixtures: 2. Mutual Diffusion.**
Final rept.,
J. M. Kincaid, M. L. de Haro, and E. G. D. Cohen. 1983, 13p
Pub. in Jnl. of Chemical Physics 79, n9 p4509-4521, 1 Nov 83.

Keywords: *Diffusion, Fluids, Hard sphere, Kinetic theory, Mixtures, Multicomponent, Reprints, Enskog theory.

The authors present a detailed description of the mutual diffusion coefficients of binary and ternary dense fluid mixtures of hard spheres, as given by the Revised Enskog Theory (RET) of van Beijeren and ERnst and the Standard Enskon Theory (SET) of Tham and Gubbins. The formulae for the diffusion coefficients, (see Part I of the series, J. Chem. Phys. 78, 2746 (1983)) involve the contact values of the equilibrium pair distribution functions and the chemical potentials, for which the Carnahan-Starling approximation is used. The formulae, which were obtained by making

an expansion in Sonine polynomials, are evaluated up to the third order and the convergence of the Sonine polynomial expansion is discussed. Except at low densities, the SET cannot be used to describe diffusion in hard-sphere mixtures, since it is in conflict with irreversible thermodynamics when either the Carnahan-Starling (CS) or exact equilibrium pair distribution functions are used.

*600,386*
**PB86-195559** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Length and Mass Div.
**Saturated Fluorescence In a Standing-Wave Laser Field.**
Final rept.,
H. K. Holt. 1984, 4p
Pub. in Physical Review A 30, n5 p2495-2498 Nov 84.

Keywords: *Fluorescence, Resonance, Standing waves, Reprints, Laser radiation.

An atom in a near-resonant standing wave laser field emits light spontaneiously from its upper level which shows a dip at resonance. The calculation gives the intensity emitted as a function of laser tuning and of the saturation parameter. The case of oppositely directed waves of unequal amplitudes is also treated.

*600,387*
**PB86-195617** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Spectroscopy and Collisional Quenching for A C2H2(V' sub 3 = 0,1,2).**
Final rept.,
J. C. Stephenson, J. A. Blazy, and D. S. King. 1984, 8p
Pub. in Chemical Physics 85, n1 p31-38 1984.

Keywords: *Acetylene, *Spectroscopy, Spectra, Excitation, Fluorescence, Reprints.

Laser excited fluorescence excitation and dispersed fluorescence spectra have been recorded for the origin and v3 = 1 and 2 levels of A C2H2. Fluorescence decay rates were obtained as a function of pressure at room temperature. The slopes of the Stern-Volmer plots gave quenching rate constants for the A C2H2 v3 = 0, 1, and 2 levels in collisions with C2H2, N2, O2, He, and Ar; the intercepts gave zero pressure fluorescence lifetimes. The results are compared to available information on acetylene spectroscopy and kinetics.

*600,388*
**PB86-195765** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Field-Dependent C-13 Chemical Shifts in Solids: A Second-Order Dipolar Perturbation.**
Final rept.,
D. L. VanderHart. 1 Feb 86, 10p
Pub. in Jnl. of Chemical Physics 84, n3 p1196-1205, 1 Feb 86.

Keywords: *Chemical shifts, *Carbon 13, Dipolar, Solids, Reprints, Nuclear magnetic resonance.

The observation of field-dependent C-13 chemical shifts in the presence of high-power proton decoupling and magic angle sample spinning (MAS) is documented. While the principal data were taken at fields of 1.4 and 4.7 T, the difference in chemical shift, in ppm, between the crystalline resonance of polyethylene and a reference resonance of solid adamantane varied as (a+bB0-2) in measurements taken at six different fields in as many laboratories. At a given field there is no dependence of the shift difference on proton resonance offset, proton rf field strength, or sample spinning speed. In rigid solids, the 'b' term in the foregoing relationship is twice as large for a methylene as for a methine carbon. Results of chemical shift measurements at two fields are reported for polyethylene, polypropylene, and three molecular solids including the normal alkane, nonadecane, which exhibits fast well-defined molecular rotation in the solid rotator phase. The observed shift differences for several kinds of carbons at 1.4 and 4.7 T agree very well with the explanation that the b term in the above expression results from a second-order energy perturbation involving the nonsecular 'C' and 'D' terms of the dipolar Hamiltonian.

*600,389*
**PB86-196003** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Length and Mass Div.
**Analytical Study of Quasi-Discrete Stark Levels In Rydberg Atoms.**
Final rept.,
D. A. Harmin. 1984, 16p
Pub. in Physical Review A: General Physics 30, n5 p2413-2428 1984.

Keywords: *Energy transfer, Atomic energy levels, Reprints, *Rydberg atoms, *Stark effect, *Excitation transfer.

A theory of nonhydrogenic Stark spectra based on the hydrogen atom is specialized to quasi-discrete levels. Core effects appear through zero-field quantum defects microliters and dipole matrix elements. Isolated and interacting Stark manifold with m=0 and 1 are examined for systems with two non-negligible microliters. A full Stark map of calculated intensities fr is presented for Li (m=0) and agrees with experiment. Pseudocrossings occur at near triple degeneracies of hydrogen-Stark states. Extensions to include ls coupling are indicated. Experimental ionization rates in He are analyzed in a companion paper by van de Water, Mariani, and Koch.

*600,390*
**PB86-196276** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Near-Threshold Measurements of the Spin Dependence of Electron-Impact Ionization.**
Final rept.,
M. H. Kelley, W. T. Rogers, R. J. Celotta, and S. R. Mielczarek. 1983, 3p
Pub. in Physical Review Letters 51, n24 p2191-2193 1983.

Keywords: *Sodium, *Polarization(Spin alignment), *Ionization, Electron irradiation, Reprints, Electron spin polarization.

The authors have measured the spin dependence of the ionization of Na up to 2eV above threshold with high precision and electron energy resolution to search for the existence of characteristic oscillations which would support the Coulomb-dipole theory of threshold ionization. The authors see no such oscillations and the results are fully consistent with the Wannier theory.

*600,391*
**PB86-196284** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Transpiration Mass-Spectrometric Analysis of Liquid KCl and KOH Vaporization.**
Final rept.,
J. W. Hastie, K. F. Zmbov, and D. W. Bonnell. 1984, 32p
Pub. in High Temperature Science 17, p333-364 1984.

Keywords: *Potassium chloride, *Potassium hydroxides, Vaporizing, Transpiration, Mass spectroscopy, Electron irradiation, Reprints, Ionization cross sections.

Existing thermodynamic functions for the equilibrium vapor species over liquid KCl and KOH are based largely on an extrapolation of data for the lower temperature solid systems together with estimated spectroscopic constants. Using a transpiration mass spectroscopic method, the authors have determined the equilibrium vapor composition in the presence of liquid over a wide range of temperature and pressure. The results for KCl are in very good agreement with the JANAF evaluation of previous work. In addition, thermodynamic data are given for the (KCl)3 trimer species for the first time. For the KoH system, the dimer species (KOH)2 is much more important than suggested by the JANAF evaluation of previous work. Thermochemical data are also reported for the KO2 species. Bond dissociation energies and entropies for the various potassium halide and hydroxide species are found to correlate well with other alkali halide systems. Evidence of temperature dependent electron impact ionization is also indicated in these results.

*600,392*
**PB86-196474** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Selection Rules for Rotational Excitation of Polyatomic Molecules by Slow Electron Impact.**
Final rept.,
G. A. Natanson. 1985, 9p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, p4481-4489 1985.

Keywords: *Atomic excitations, *Molecular rotation, *Particle collisions, Reprints.

Fundamental selection rules for rotational excitation of polyatomic molecules by slow electron impact have been derived as a result of conservation of molecular symmetry with respect to feasible permutations of nuclei. Special attention is given to an analysis of selection rules for molecules having the same dynamical permutation-inversion group of their free rotating rigid models with the only difference being that elements of the group represent feasible permutations in different ways. Asymmetric tops H2O, H2CO and C2H4 give a typical example.

*600,393*
**PB86-196490** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Reactions of Iron (3): Porphyrins with Peroxyl Radicals Derived from Halothane and Halomethanes.**
Final rept.,
D. Brault, and P. Neta. 1984, 6p
Pub. in Jnl. of Physical Chemistry 88, n13 p2857-2862 1984.

Keywords: *Electron transfer, *Electrochemistry, Porphyrins, Halothane, Reprints, *Cytochrome.

The reactions of haloalkane derived peroxyl radicals with ferric deuterophyrins in aerated acidic or alkaline aqueous 2-propanol solutions are investigated by means of pulse radiolysis. CC13O2, CHCl2O2, CH2ClO2 and CF3CHlO2 radicals (the latter one being derived from the anesthetic agent halothane, CF3CHC1Br) are found to oxidize the ferric porphyrins with reaction rate constants ranging between 6 times 10 to the seventh power and 2.6 times 10 to the eight power M-1s-1. In keeping with an electron transfer mechanism, the spectrum of the oxidized ferric porphyrin does not depend on the nature of the peroxyl radicals. Also, the rate constant for the reaction of CCl3O2 radicals with ferric porphyrins is lowered by a factor greater than or equal to 20 when experiments are performed in the less polar solvents neat 2-propanol and neat carbon tetrachloride. The spectrum of the oxidized ferric porphyrin depends on pH with large changes around pH = 2.3 which are attributed to the protonation of an alkoxide ligand of the iron ion.

*600,394*
**PB86-196508** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.
**Comparative Rate Method for the Study of Unimolecular Fall-Off Behavior.**
Final rept.,
W. Braun, J. R. McNesby, and M. D. Scheer. 1984, 5p
Pub. in Jnl. of Physical Chemistry 88, n9 p1846-1850 1984.

Keywords: High temperatures, Comparison, Reprints, *Unimolecular decomposition, Fall off behavior.

A comparative method was applied to a high temperature fast flow reactor to determine relative kinetic parameters for the two channel decomposition of cyclobutanone in the fall-off regime. The applicability of the method to such non-thermally-equilibrated systems was assessed and found to be generally useful over wide range of conditions. The measurements could, therefore, be used as a quantitative diagnostic tool for sensing unimolecular fall-off behavior in a number of heat bath gases. A simple stepladder collisional activation--deactivation model was used to determine the energy transferred per collision. The values obtained for the heat bath gases; He, Ar, SiF4 and SF6 were 3.0, 2.0, 3.5, and 4.0 kcal/mol respectively. These are small multiples of RT and very small fractions of the activation energy indicating that weak collisions must be a dominant feature of reaction types represented by the decomposition of cyclobutanone.

*600,395*
**PB86-196839** Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Laser Photodetachment Measurement of the Electron Affinity of Atomic Oxygen.**
Final rept.,
D. M. Neumark, K. R. Lykke, T. Andersen, and W. C. Lineberger. Sep 85, 3p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review A 32, n3 p1890-1892 Sep 85.

Keywords: Reprints, *Atomic oxygen, *Electron affinity, *Photodetachment.

The electron affinity of atomic oxygen, an important calibration standard in negative-ion photoelectron spectroscopy, has been determined by tunable-laser photodetachment in a coaxial laser-ion-beam spectrometer to be 11 784.645 + or - 0.006 per cm. In addition, the spin-orbit splitting between the 2P 3/2 and 2P 1/2 states of 0- was found to be 177.13 + or - 0.05 per cm.

*600,396*
**PB86-200219** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Search for the Prewetting Line.**
Final rept.,
J. W. Schmidt, and M. R. Moldover. 15 Apr 86, 6p
Contract NASA-H-27954-B
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Chemical Physics 84, n8 p4563-4568, 15 Apr 86.

Keywords: *Wetting, Polarimetry, Reprints, Liquid-vapor interfaces, Ellipsometry, Cyclohexane/methyl-perfluoro, Isopropyl alcohol.

The paper describes efforts to locate the prewetting line in a binary liquid system (isopropanol-perfluoromethylcyclohexane) at the vapor-liquid interface. We placed tight upper bounds on the temperature separation (0.2K) between the prewetting line and the line of bulk liquid phase separation. We did not detect the prewetting line in systems at equilibrium. Experimental signatures indicative of the prewetting line occurred only in nonequilibrium situations. Several theories predict that the adsorption of one of the components (the fluorocarbon, in this case) at the liquid-vapor interface should increase abruptly, at a temperature sightly above the temperature at which the mixture separates into two liquid phases. A regular solution calculation indicates that the prewetting line should have been easily detectable with the instruments used in the experiment. Significant features of the experiment are: (1) low-gradient thermostating, (2) in situ stirring, (3) precision ellipsometry from the vapor-liquid interface, (4) high resolution differential index of refraction measurements using a novel cell design, and (5) computer control.

*600,397*
**PB86-200227** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Time-Resolved Measurements of Vibrational Relaxation at Surfaces.**
Final rept.,
M. P. Casassa, E. J. Heilweil, J. C. Stephenson, and R. R. Cavanagh. 1986, 9p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 38, p257-265 1986.

Keywords: *Surfaces, *Molecular relaxation, Semiconductor(Materials), Silicon dioxide, Zinc oxides, Ion exchange resins, Time measurement, Reprints, Time dependence, Pico second pulses, Hydroxyl compounds.

Time-resolved measurements of optically induced transients on surfaces are reported. Room temperature vibrational energy relaxation rates for OH groups on the insulators SiO2 and zeolite ZSM-5 are found to be comparable (approx. equal to 10 to the 10th power/s). The relaxation rate for optically induced transients on the semiconductor surface ZnO appears to reflect the influence of conduction bands in the 8 micrometer spectral region.

*600,398*
**PB86-200391** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Model Simulation of Chemical Reaction in a Diatomic Crystal. 1. Energy Exchange in Rapid Exothermic Dissociation.**
Final rept.,
D. H. Tsai, and S. F. Trevino. 1984, 4p
See also PB86-200409. Sponsored by American Physical Society, New York.
Pub. in Proceedings of the Americal Physical Society Topical Conference on Shock Waves in Condensed Matter, Santa Fe, NM., July 18-21, 1983, p629-632 1984.

Keywords: *Dissociation energy, Exothermic reactions, Diatomic molecules, Computerized simulation, Energy transfer, Explosions, *Diatomic crystals.

In the work the author describes the results of a molecular dynamics simulation of a rapid exothermic reaction in the solid state. The model consists of 256 particles arranged in pairs as diatomic molecules in a three-dimensional cube with periodic boundary conditions. The particles interact through a pairwise potential such that the diatomic molecules are metastable with respect to the dissociated state. The dynamics of energy transport (potential and kinetic) during the dissociation process is studied as are the conditions prerequisite to initiation.

*600,399*
**PB86-200409** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Reactor Radiation Div.
**Model Simulation of Chemical Reaction in a Diatomic Crystal. 2. Kinetics of Equilibrium Chemistry.**
Final rept.,
S. F. Trevino, and D. H. Tsai. 1984, 4p
See also PB86-200391. Sponsored by American Physical Society, New York.
Pub. in Proceedings of the American Physical Society Topical Conference on Shock Waves in Condensed Matter, Santa Fe, NM., July 18-21, 1983, p633-636 1984.

Keywords: Chemical equilibrium, Computerized simulation, Heat of reaction, *Chemical reaction kinetics, *Diatomic crystals.

The properties of a model which exhibits equilibrium chemical reactions are reported. It is shown that the kinetics produced is consistent with established thermodynamic considerations. Further, at constant pressure, the relation between the Arrhenius energy of reaction, the potential energy change upon reaction, and the work done due to the volume change upon reaction, is satisfied.

*600,400*
**PB86-200433** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Quenching of Resonant Laser-Driven Ionisation at High Buffer Gas Pressures.**
Final rept.,
W. T. Hill. 1986, 10p
Sponsored by Maryland Univ. at Baltimore, and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Physics B: At. Mol. Phys. 19, p359-368 1986.

Keywords: *Barium, *Gas ionization, Atomic energy levels, Helium, Argon, Reprints, Laser-produced plasma, Quenching.

The modification of ion production efficiency via resonant laser-driven ionization in the presence of high buffer gas atmospheres has been experimentally investigated in a barium vapor. The populations of several energy levels of neutral and singly ionized Ba were measured as a function of both helium and argon pressures by the time-resolved hook technique. The behaviors of He and Ar are quite distinct. The percentage of ionization decreased monotonically from nearly 100% to less than 10% as the helium pressure was increased from 0.01 to 1 atm, while no quenching was observed in 1 atm of Ar. These observations are consistent with a quenching mechanism based in part on cooling of the 'hot' electrons through momentum-changing elastic collisions with the He atoms.

*600,401*
**PB86-200680** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Angular Momentum Distribution of Electrons in Above-Threshold Ionization.**
Final rept.,
K. Rzazewski, and R. Grobe. Mar 86, 4p
Sponsored by Joint Inst. for Lab. Astrophysics, Boulder, CO.
Pub. in Physical Review A 33, n3 p1855-1858 Mar 86.

Keywords: Photoelectrons, Gas ionization, Reprints, *Multiphoton ionization, *Multi-photon processes, *Hydrogen atoms, Laser radiation.

The authors examine a quantum optical model describing absorption of photons above an ionization threshold in multiphoton ionization. They calculate 12-photon ionization of the hydrogen atom by a strong, linearly polarized laser pulse. The angular momentum distribution of photoelectrons in the consecutive peaks depends on the intensity of the laser but reveals the prescence of only a few of the lowest angular momenta. No 'peak switching' is observed, but a finite-number-of continua model becomes unstable at an intensity of about 0.001 a.u.

*600,402*
**PB86-200706** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Relationship of the Unweighted Rosenbluth Walk to a Polymer Chain at the Theta Point.**
Final rept.,
C. M. Guttman. Mar 86, 5p
Pub. in Macromolecules 19, n3 p833-837 Mar 86.

Keywords: Reprints, *Polymer chains, *Rosenbluth walk, *Theta point.

It is shown that the unweighted Rosenbluth and Rosenbluth (R-R) chains (sometimes called the 'true' self-avoiding walk) can be viewed as polymer chains at the theta point where only second-order cluster-like terms have been included in the partition function. A modified weighting function for the R-R model is proposed that includes only such second-order cluster terms. Such a polymer chain is shown to show normal polymer chain behavior, i.e., chain expansion, a theta point, and chain collapse. It is suggested that by comparing the results of studies on these chains with those obtained by a normal R-R weighting procedure one should be able to accurately assess the contributions of third-order and higher order cluster terms to polymer chain properties.

*600,403*
**PB86-200722** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Study of Thermal Depolarization of Polyvinylidene Fluoride Using X-ray Pole-Figure Observations.**
Final rept.,
A. J. Bur, J. D. Barnes, and K. J. Wahlstrand. Apr 86, 10p
Pub. in Jnl. of Applied Physics 59, n7 p2345-2354 Apr 86.

Keywords: *Depolarization, Aging tests(Materials), Piezoelectricity, Pyroelectricity, Dipole, Reprints, *Vinylidene fluoride polymers.

Measurements of piezoelectric and pyroelectric activity, density, and x-ray pole figures were used to study the effect of thermal aging on the state of polarization in polyvinylidene fluoride. A rolled and poled beta-phase specimen of polyvinylidene fluoride was subjected to thermal aging which consisted of temperature cycling between room temperature and successively higher maximum temperatures T (max), where T (max) ranged from room temperature to 164 deg C. We found that the room temperature piezo and pyroelectric activity decreased linearly as a function of T (max) from 75 deg C to 164 deg C at which temperature the specimen had 30% of its original activity; a linear extrapolation of these data to zero activity yielded a temperature T sub c = 207 deg C. Based on these data, we propose a model which describes the state of polarization in polyvinylidene fluoride and from which we calculate the fraction of dipoles in the crystalline state contributing to the polarization.

*600,404*
**PB86-200755** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

**Low Vapor Density Measurements by Saturated Absorption.**
Final rept.,
M. Raab, and J. J. Snyder. 1983, 7p
Pub. in Proceedings of SPIE - Laser-Based Ultrasensitive Spectroscopy and Detection V, San Diego, CA., August 23-24, 1983, p99-105.

Keywords: Sodium, Spectral lines, Absorption, Sensitivity, *Low density gases, *Sodium vapor, Laser spectroscopy.

Saturation spectroscopy and polarization spectroscopy were applied to low density measurements in sodium vapor. Using the D sub 1 and D sub 2 lines a sensitivity was achieved to defect a minimum number of a few thousand atoms.

*600,405*
**PB86-200979** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Spectrum and Energy Levels of Singly Ionized Cesium: 1. Revision and Extension of the Cs II Energy Levels.**
Final rept.,
C. J. Sansonetti, and K. L. Andrew. Mar 86, 12p
Pub. in Jnl. of the Optical Society of America B 3, n3 p386-397 Mar 86.

Keywords: *Atomic energy levels, Hyperfine structure, Ionization, Reprints, *Cesium ions.

The experimentally determined energy levels of Cs II have been revised and extended based entirely on recent observations of the spectrum. Most observed lines have been classified as transitions between 118 even and 167 odd energy levels. Of these 285 levels, 233 have not been previously reported. All the levels have been assigned designations in the jK coupling notation based on theoretical interpretation of the structure and empirical factors. Hyperfine splitting constants are given for 167 levels. By fitting polarization and extended Ritz formulas to selected Rydberg series, the Cs II ionization energy has been determined to be 186 777.4(5)/cm.

*600,406*
**PB86-200987** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Laser-Driven Ionization of Cs and Absorption Spectrum of Resultant Cs (1+) Vapor.**
Final rept.,
T. J. McIlrath, J. Sugar, V. Kaufman, D. Cooper, and W. T. Hill. Mar 86, 5p
Contract AFOSR-ISSA-850033, Grant NSF-CPE84-17933
Sponsored by National Science Foundation, Washington, DC., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of the Optical Society of America B 3, n3 p398-402 Mar 86.

Keywords: *Gas ionization, Absorption spectra, Optical pumping, Reprints, *Cesium ions, Laser-produced plasma, Laser radiation, Dye lasers.

By pumping the 6s-7p line of neutral cesium at 4593 with a flash-pumped dye laser, the authors obtained about 80% ionization in a heat-pipe-generated Cs vapor. An absorption spectrum of Cs (1+) was then obtained, showing the 5p(6) - 5p(5)nd and ns Rydberg series both below and above the 5p(5) doublet P(3/2) threshold. Effects of channel mixing are seen in the broadening of the nd series members above threshold and in the anomolous intensity behavior below. This strong interaction is reflected in the Lu-Fano plot shown for these data.

*600,407*
**PB86-201001** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Absolute Physical Quantities.
**Longitudinal Ramsey-Fringe Spectroscopy in a Calcium Beam.**
Final rept.,
J. J. Snyder, J. Helmcke, and D. Zevgolis. 1983, 7p
Pub. in Applied Physics B-Photophysics and Laser Chemistry 32, n1 p25-31 1983.

Keywords: *Calcium, *Frequency standards, Atomic beams, Reprints, *Laser spectroscopy, *Ramsey fringes.

For ultra-high resolution applications such as optical frequency standards, the value of thermal sources such as atomic beams is currently limited by second-order Doppler broadening. The use of a longitudinal interaction geometry in which an atomic beam crosses the counter-propagating laser fields at a shallow angle is able to reduce second-order Doppler broadening to an insignificant level as well as to provide long interaction times without the necessity of large diameter optical beams. We have analyzed the geometry for the case of the long-lived calcium intercombination line, and conclude that when combined with pulsed (Ramsey) excitation, the longitudinal interaction geometry could be used with a thermal calcium beam to create an optical frequency standard with a reproducibility of the order of 10 to the minus 14th power for a few seconds' averaging time. Our initial experimental results have demonstrated the first use of the longitudinal geometry.

*600,408*
**PB86-201043** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Auger Spectroscopy of Solid Surfaces: Electron Versus Ion Excitation.**
Final rept.,
J. A. D. Matthew. 1982, 10p
Pub. in Proceedings of International Workshop Inelastic Ion-Surface Collisions, Middelfart, Denmark, September 21-24, 1982, Phys. Scr. T6, p79-88 1983.

Keywords: *Surfaces, *Auger electron spectroscopy, Band theory.

Auger transitions involving outer electrons in free atoms and in solids are compared with particular reference to L(23) deexcitation in elements Na to Si. Under electron or X-ray excitation the elemental solid state spectra are band-like in character with breadth twice that of the conduction valence band, and a shape determined in detail by matrix element, surface and electronic relaxation effects. This is in strong contrast to the L(23)VV spectrum of Cu which is quasi-atomic in character and the M(45)VV spectrum of various Ag alloys which show mixed atomic-band like behavior. Under ion excitation a superposition of a solid state spectrum and an excited atom spectrum is observed. Various theories of the origin of the quasi-atomic spectrum are considered, and attempts are made to account for the energies in the atomic spectrum and the relative intensities of atomic and solid state features. Calculations of the detailed motions of atoms in the surface region following inner shell ionization are reviewed, and the sensitivity of atomic yield to inner core lifetime and the angle of incidence of the ion beam is discussed.

*600,409*
**PB86-201449** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
**Interaction of Vibrating H Atoms on the Surface of Platinum Particles by Isotope Dilution Neutron Spectroscopy.**
Final rept.,
J. J. Rush, R. R. Cavanagh, R. D. Kelley, and J. M. Rowe. 15 Nov 85, 3p
Pub. in Jnl. of Chemical Physics 83, n10 p5339-5341, 15 Nov 85.

Keywords: *Platinum, *Surfaces, Particles, Neutron spectroscopy, Catalysts, Reprints, *Hydrogen atoms.

No abstract available.

*600,410*
**PB86-201456** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Aluminum. 1. Measurement of the Relative Enthalpy from 273 to 929 K and Derivation of Thermodynamic Functions for Al(s) from 0 K to Its Melting Point.**
Final rept.,
D. A. Ditmars, C. A. Plint, and R. C. Shukla. Sep 85, 17p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Natural Sciences and Engineering Research Council of Canada, Ottawa (Ontario).
Pub. in International Jnl. of Thermophysics 6, n5 p499-415 Sep 85.

Keywords: *Aluminum, *Enthalpy, Polycrystalline, Specific heat, Thermodynamics, Quartz, Reprints, Calorimetry.

The relative enthalpy of pure, polycrystalline aluminum (NBS Standard Reference Material 44f, for the freezing point of aluminum on IPTS-68) has been measured over the temperature range 273 to 929 K. The enthalpy measurements were made in a precision isothermal phase-change calorimeter and are believed to have an inaccuracy not exceeding 0.2 percent. Pt-10Rh alloy and quartz glass were used as the encapsulating materials. The enthalpy data for Al(s) and SiO2(l) have been fitted by the method of least squares with cubic polynomial functions of temperature. Heat capacity data for Al(s), derived from these polynomials, have been smoothly merged using a spline technique to the most reliable low-temperature heat capacity data for Al(s) below 273 K. The merged data are compared with corresponding data from the literature as well as with published critical compilations of heat capacity data for Al(s). A new table of thermodynamic functions for Al(s) has been derived. A theoretical interpretation of the results appears in a companion paper.

*600,411*
**PB86-202397** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Spectroscopy and Reaction Kinetics of Photolytically Generated Fe(CO)x (x=2,3,4).**
Final rept.,
A. J. Ouderkirk, T. A. Seder, and E. Weitz. 1984, 6p
Sponsored by SPIE-The International Society for Optical Engineering, Bellingham, WA.
Pub. in Proceedings of the SPIE International Conference on Applications of Lasers to Industrial Chemistry, Los Angeles, CA., January 24-25, 1984, v458 p148-153.

Keywords: *Metal carbonyls, *Reaction kinetics, Adsorption, Infrared spectra, *Iron carbonyls.

An apparatus for the gas phase infrared spectroscopic detection of coordinatively unsaturated metal carbonyls is described. Coordinatively unsaturated species are produced by UV photolysis. Infrared spectra of coordinatively unsaturated iron carbonyls are reported for the carbonyl stretch region. Rate constants for the reaction of Fe(CO)3 and Fe(CO)4 with Co are also reported. The photophysics of Fe(CO)x formation is discussed.

*600,412*
**PB86-202819** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**4d-Photoabsorption of Barium: A View of Shell Collapse vs Contraction.**
Final rept.,
T. B. Lucatorto, T. J. McIlrath, W. T. Hill, and C. W. Clark. Dec 82, 18p
Pub. in Proceedings of the AIP (American Institute of Physics) Conference on X-ray and Atomic Inner-Shell Physics, Eugene, OR., August 22-27, 1982, 94, p584-601.

Keywords: *Barium, Ionization, Photochemical reactions, Contraction, Atomic orbitals, *Photoabsorption, Barium ions, Configurations.

Ba with Z=56 is at the edge of 4f collapse; neutral ground state atoms with Z<56 have 4f orbitals which are hydrogenic with (r sub (av) approx = 17a sub 0) while elements with Z>56 have a 'collapsed' 4f orbital with (r sub (av) approx = 1a (sub 0). Since the 4d orbital is collapsed (r sub (av) approx = 1a (sub 0) the nature of the 4d-absorption is expected to depend critically on whether the 4f orbital can be considered 'collapsed' or not. Using a laser technique to prepare dense homogenous columns of Ba(1+) and Ba(2+) the authors have obtained the 4d photoabsorption spectra of Ba, Ba(1+) and Ba(2+). The technique thus allows the authors to observe the effects on the 4f orbitals of the increased nuclear attraction experienced in the absence of screening by the 6s electrons. It is found that exchange effects are critically important in configurations of the type 4d(9)4f, and that progressive 'contraction' rather than 'collapse' is a more appropriate description under such conditions.

*600,413*
**PB86-204567** Not available NTIS
American Chemical Society, Washington, DC.
**Journal of Physical and Chemical Reference Data, Volume 15, Number 1, 1986.**
Quarterly rept.
c1986, 451p
See also PB86-204575 through PB86-204609, and PB86-165560. Prepared in cooperation with American

Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research, Microwave spectra, Water, Heavy water, Thermodynamic properties, Triplet state, Interstellar gas, Molecular clouds, Forbidden transitions.

Contents:
- Triplet-Triplet absorption spectra of organic molecules in condensed phases;
- Recommended rest frequencies for observed interstellar molecular microwave transitions-1985 revision;
- New international formulations for the thermodynamic properties of light and heavy water;
- Forbidden lines in n(s, sup 2)n(p sup k) ground configurations and nsnp excited configurations of beryllium through Molybdenum atoms and ions;
- Cumulative listing of reprints and supplements.

*600,414*
**PB86-204575** Not available NTIS
Notre Dame Univ., IN. Radiation Chemistry Data Center.
**Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases,**
I. Carmichael, and G. L. Hug. c1986, 250p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n1 p1-250 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Triplet state, Absorption spectra, Condensing, Photolysis, Organic compounds, Triplet-triplet interactions, Triplet production, Pulse radiolysis, Extinction coefficients.

A compilation of spectal parameters associated with triplet-triplet absorption of organic molecules in condensed media is presented.

*600,415*
**PB86-204591** Not available NTIS
Maryland Univ., College Park. Inst. for Physical Science and Technology.
**New International Formulations for the Thermodynamic Properties of Light and Heavy Water,**
J. Kestin, and J. V. Sengers. c1986, 16p
Prepared in cooperation with National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
Included in Jnl. of Physical Chemical Reference Data, v15 n1 p305-320 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Heavy water, *Water, *Thermodynamic properties, Equations of state.

The general assembly of the international association for the properties of steam (IAPS), meeting at the 10th international conference on the properties of steam in Moscow in September 1984, adopted new formulations for the thermodynamic properties of fluid H2O and D2O. The new formulations have been designated as the IAPS Formulation 1984 for the thermodynamic properties of ordinary water substance for scientific and general use and the IAPS formulation 1984 for the thermodynamic properties of heavy water substance. In the paper the authors present and discuss these new formulations.

*600,416*
**PB86-204609** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Forbidden Lines in n(s sup 2)n(p sup k) Ground Configurations and nsnp Excited Configurations of Beryllium through Molybdenum Atoms and Ions,**
V. Kaufman, and J. Sugar. c1986, 105p
Included in Jnl. of Physical and Chemical Reference Data, v15 n1 p321-435 1986. Available from American Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: Line spectra, Magnetic dipoles, Ground state, Transition probabilities, Wavelengths, Tables(Data), *Forbidden transitions, Energy-level transitions, Excited states.

Observed and predicted wavelengths of magnetic dipole lines arising within ground configurations of the type n(s sup 2)n(p sup k)(n=2 and 3, k=1 to 5) are compiled. For n=2 the compilation includes the elements B through Kr, and for k=5 it extends to Mo. For n=3 Al through Mo are included. In addition the 2s2p excited configuration of the Be i isoelectronic sequence for Be through Kr and 3s3p of the Mg sequence for Mg through Mo are included. For each line the authors give a calculated value for the transition probability obtained mainly from the Dirac-Fock method or from the use of scaled radial integrals. The calculated wavelengths are obtained from known energy levels or from levels derived from scaled radial integrals. A small group of electric quadrupole lines seen in astronomical sources are included. The list contains 1660 predicted wavelengths in the range 100 A to 25.9 mm and 406 observed wavelengths in the range 325 A to 609 micrometers.

*600,417*
**PB86-207164** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Metastability in the H2O and D2O Systems at High Pressure.**
Final rept.,
G. J. Piermarini, R. G. Munro, and S. Block. 1984, 4p
Pub. in Proceedings of AIRAPT International High Pressure Conference (9th), Albany, NY., July 24-29, 1983, p25-28 1984.

Keywords: *Heavy water, *Water, Deuterium compounds, Metastable state, High pressure.

The pressure and temperature parameters which delineate the equilibrium thermodynamic stability fields of the liquid, VI and VII phases, including the triple point, were measured for the H2O and D2O systems over the pressure range, 0.8 to 2.4 GPa, and the temperature interval, 20 to 135 C. The phenomenon of metastability associated with the liquid-VII phase boundary was observed during the work; and, subsequently, a metastable extension of the coexistence curve was determined, from the liquid-VI-VII triple point down to 20 C, for both H2O and D2O. The measurements were made by optical polarizing microscopy in conjunction with a diamond anvil cell equipped with a miniature resistance coil heating element. Pressures were measured by the ruby fluorescence method.

*600,418*
**PB86-208410** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Internal States Distributions of NO Thermally Desorbed from Pt(111): Dependence on Coverage and Co-Adsorbed CO.**
Final rept.,
D. A. Mantell, R. R. Cavanagh, and D. S. King. 1986, 12p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Chemical Physics 84, n9 p5131-5142, 1 May 86.

Keywords: *Desorption, *Nitric oxide, Lasers, Platinum, Polarization, Rotational state, Reprints.

The distribution of population in the internal energy levels of nitric oxide thermally desorbed from Pt(111) has been probed using laser excited fluorescence. The observed rotational distributions have been found to follow the Boltzmann distribution function, independent of NO coverage or the presence of pre- or post-adsorbed CO. Under all conditions of NO desorption, the observed NO was characterized by a temperature (0.95 + or - 0.05) times the surface temperature. No evidence of a preferred alignment of the rotational angular momentum vectors was observed, nor was there any difference between the two spin-orbit multiplets beyond that associated with the rotational temperature.

*600,419*
**PB86-208444** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Transpiration Mass Spectrometry - A New Thermochemical Tool.**
Final rept.,
J. W. Hastie, and D. W. Bonnell. 1984, 51p
Sponsored by NATO Advanced Study Inst., Oslo (Norway).
Pub. in NATO Advanced Study Institute Series 119, p183-233 1984.

Keywords: Sampling, Mass spectrometry, Pressure measurements, Sodium chloride, Sodium sulfate, Transpiration, Reprints, *Alkali vapor transport, *Electron impact ionization.

Classical vaporization methods such as transpiration and Knudsen or Langmuir effusion have been limited because they do not establish the molecular identity of transport species or because low pressures are necessary to make effusion measuremenets. The authors have developed a new technique--Transpiration Mass Spectrometry (TMS)--that overcomes both of these limitations by combining the basic features of transpiration and molecular beam mass spectrometry. With this technique, it is possible to sample reactive gases directly from high-temperature (to 1500 deg C), high-pressure (to 10 atm) atmospheres for quantitative characterization with a mass spectrometer. The accuracy of thermochemical data obtained by the TMS method is competitive with that of established lower dynamic range techniques. Examples of application to vaporization of complex silicate slags, glasses, and minerals are considered. Implications and precautions resulting from cooling effects during the sampling process are also discussed.

*600,420*
**PB86-208451** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Analysis of Submicrometer Particles by Sequential AEM and LAMMA.**
Final rept.,
E. B. Steel, D. S. Simons, J. A. Small, and D. E. Newbury. 1984, 3p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Army Materials and Mechanics Research Center, Watertown, MA.
Pub. in Proceedings of Annual Conference on Microbeam Analysis Society (19th), Bethlehem, PA., July 16-20, 1984, Microbeam Analysis-1984, p27-29.

Keywords: *Particles, AEM, LAMMA, Submicrometer.

No abstract available.

*600,421*
**PB86-212818** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Absolute Rate Coefficients for Methyl Radical Reactions by Laser Photolysis, Time-resolved Infrared Chemiluminescence: CD3 + HX yields CD3H + X (X=Br,I).**
Final rept.,
D. J. Donaldson, and S. R. Leone. 1986, 6p
Grants NSF-CHE79-11340, NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Physical Chemistry 90, n5 p936-941 1986.

Keywords: *Chemiluminescence, Hydrogen bromide, Hydrogen iodide, Photolysis, Deuterium compounds, Reprints, *Chemical reaction kinetics, *Methyl radicals, Excimer lasers.

Absolute rate coefficients are reported for the room temperature reactions of deuterated methyl radicals with HI and HBr, CD3 + HI(HBr) -> CD3H + I(Br). Excimer laser photolysis of CD3I is used to generate methyl radicals, and time-resolved infrared chemiluminescence from the CH stretch of the CD3H products is detected to follow the time evolution of the reaction. The rate constants obtained in this manner are: (7.7 + or - 0.7) x 10 to the 12th power cc/molecule s for CD3 + HI and (4.7 + or - 0.4) x 10 to the 12th power cc/molecule s for CD3 + HBr. These rate constants are considerably greater than earlier, indirectly-measured values and indicate that the activation energy for these light-atom transfer reactions is lower than previously believed.

*600,422*
**PB86-212834** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Resonant Photoionisation of Hydrogen Atom in Intense Magnetic Fields.**
Final rept.,
S. K. Bhattacharya, and S. I. Chu. 1985, 6p
Sponsored by Department of Energy, Washington, DC., Alfred P. Sloan Foundation, New York, and Army Research Office, Research Triangle Park, NC.
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, n10 pL275-L280, 28 May 85.

Keywords: Reprints, *Autoionization, *Photoionization, *Hydrogen atoms, High magnetic field research.

A complex quasi-energy approach is presented for accurate treatment of photo-ionization of the H atom in strong magnetic fields. The autoionizing resonances near the first two excited Landau thresholds are determined by the complex-coordinate coupled-Landau-channel method. Detailed resonant photoionization cross sections and asymmetric line shapes are reported for the case of B=4.7 x 10 to the 9th power G.

*600,423*

**PB86-212859** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Flowing Afterglow Negative Ion Photoelectron Spectroscopy of Dirhenium: Evidence for Multiple Bonding in Re2 and Re2 (1-).**
Final rept.,
D. G. Leopold, T. M. Miller, and W. C. Lineberger. 1986, 2p
Grants NSF-CHE83-16628, NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of the American Chemical Society 108, p178-179 1986.

Keywords: *Chemical bonding, Dimers, Metals, Anions, Reprints, *Dirhenium, *Flowing afterglow, Photoelectron spectra, Photoelectron spectroscopy.

The authors report the first gas phase spectroscopic study of a third row open d-shell transition metal dimer. The low-lying electronic states of Re2 were probed by negative ion photoelectron spectroscopy of Re2(1-), prepared from Re2(CO)10 in a flowing afterglow ion source. Results indicate a Re2 electron affinity of 1.571 + or - 0.008 eV, and fundamental vibrational frequencies of 340 + or - 20/cm for Re2 and 320 + or - 15/cm for Re2. These frequencies imply high vibrational force constants which are strongly indicative Of multiple metal-metal bonding in both the neutral and anionic dimers.

*600,424*

**PB86-212867** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Ab Initio Calculations of Low-Energy Electron Scattering by HCN Molecules: Dependence on Internuclear Distance in Linear Geometry.**
Final rept.,
A. Jain, and D. W. Norcross. 15 Jan 86, 6p
Contract DOE-EA-77-A-01-6010
See also PB86-102977. Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Chemical Physics 84, n2 p739-744, 15 Jan 86.

Keywords: *Hydrogen cyanide, Bonding, Anions, Resonance, Band spectra, Electron scattering, Reprints, *Electron-molecule collisions, Molecular ions.

Low-energy electron scattering with HCN molecules is studied in the SEP (static-exchange plus parameter-free polarization potential) model as a function of both bond (CH and CN) stretches. A doublet Pi resonance at the equilibrium geometry behaves very similarly to the CO doublet Pi resonance as the CN bond is stretched; the corresponding HCN(-1) (doublet Pi) potential surface seems to cross the neutral curve (HCN singlet Sigma (+1) around 2.9 a.u. of CN distance. In (supZ)Sigma symmetry, where no shape resonance is present at equilibrium geometry, a broad resonance appears when the CH or CN bonds are stretched well beyond the equilibrium position; the former appears to cross the (doublet Sigma (+1) curve at about 2.8 a.u., i.e., just below the H + CN(-1) asymptote, the latter to approach the neutral curve much more slowly and tangentially. Structure interpreted as a Pi resonance in vibrational excitation, and as necessarily of Sigma character in dissociative attachment to the lowest anion-neutral asymptote, can be explained as due to the mixing of the lowest linear doublet Pi and (sup 2)Sigma resonances through bending (the Renner-Teller effect) and the peculiarity (cusp behavior) associated with anion-neutral curve crossings in polar molecules.

*600,425*

**PB86-212875** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Angularly Resolved Vibrational Excitation in Na2-He Collisions.**
Final rept.,
E. Gottwald, A. Mattheus, K. Bergmann, and R. Schinke. Jan 86, 8p
Pub. in Jnl. of Chemical Physics 84, n2 p756-763 Jan 86.

Keywords: *Helium, *Sodium, Excitation, Energy transfer, Molecular vibration, Reprints, *Molecule-molecule collisions.

The paper reports angle-resolved measurements of V(subi)=0->V(Sub f)=1 vibrational transitions in Na2-He collisions at an energy of 90 MeV. The agreement with calculated cross sections using an ab initio surface is good, both in the angular variation of the cross section as well as with respect to its magnitude relative to the vibrationally elastic process. The calculated v(sub i)=0,j(sub i)=0 ->v(sub f)=1, j(sub f) differential cross sections are discussed in some more detail. They show structure, in addition to the rainbow oscillations, related to the fact that the vibrational transition probability vanishes for a specific approach angle.

*600,426*

**PB86-212891** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Saturation of an Atomic Transition by a Phase-Diffusing Laser Field.**
Final rept.,
M. W. Hamilton, D. S. Elliott, K. Arnett, and S. J. Smith. Jan 86, 4p
Contract DOE-EA-77-A-01-6010
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A 33, nl p778-781 Jan 86.

Keywords: *Electron transitions, Resonance, Atomic energy levels, Reprints, Sodium atoms, Laser radiation.

The authors have studied the effect of well-characterized laser frequency fluctuations on the saturation of an atomic resonance in a double optical resonance experiment. The peak-height asymmetry of the observed Autler-Townes signal was reversed at small detunings when the shape of the saturating laser power spectrum was changed from nearly Gaussian to nearly Lorentzian. The behavior agrees qualitatively with theoretical calculations and also with previous observations using lasers without such well-characterized fluctuations.

*600,427*

**PB86-212917** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Comment on Rotational Energy Surfaces and High-J Eigenvalue Structure of Polyatomic Molecules.**
Final rept.,
G. A. Natanson. 1986, 3p
Pub. in Jnl. of Chemical Physics 84, n9 p5216-5218, 1 May 86.

Keywords: *Molecular structure, Assymmetry, Eigenvalues, Reprints, *Polyatomic molecules.

The main aim of these comments is to reveal some defects of the labeling scheme proposed by Harter and Patterson. It is shown that quasi-degenerate doublets found by these authors in the calculated spectra of an asymmetric-top molecule are nothing but K-doublets well known to molecular spectroscopists. The use of the nonstandard notation merely disguised this fact.

*600,428*

**PB86-212925** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Experimental Proof of an (Absolute Value of Delta m) << j Propensity Rule in Rotationally Inelastic Differential Scattering.**
Final rept.,
A. Mattheus, A. Fischer, G. Ziegler, E. Gottwald, and K. Bergmann. 1986, 4p
Pub. in Physical Review Letters 56, n7 p712-715, 17 Feb 86.

Keywords: Differential cross sections, Sodium, Neon, Optical pumping, Reprints, *Atom molecule interactions, MeV range 100-1000.

The first measurement of a fully state-selected differential cross section in atom-molecule collisions is reported. A realistic estimate for the relative contribution of collision processes with (absolute value of delta m)>0 gives an upper limit of 10%.

*600,429*

**PB86-212933** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Nascent Rotational Distribution of the Minor v=0 Channel in the N2(1+) Product of the AR(1+)N2 Charge Transfer Reaction at Near Thermal Energy.**
Final rept.,
G. H. Lin, J. Maier, and S. R. Leone. 1986, 4p
Contract NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Chemical Physics Letters 125, n5/6 p557-560, 18 Apr 86.

Keywords: Chemical reactions, Reprints, *Ion-molecule collisions, *Nitrogen ions, *Argon ions, Flowing afterglow, Charge transfer.

An improved ion beam apparatus is used to study the nascent state distribution of products in the Ar(1+)+N2 charge transfer reaction at 0.28 eV collision energy. The rotational distribution of the minor nu=0 vibrational channel under single-collision conditions can be characterized by a Boltzmann distribution with a temperature T=710 + or - 70 K, compared to the higher temperature of 980 + or - 10 K for the major nu=1 vibrational pathway. It is suggested that these two vibrational channels are formed by different reaction mechanisms, most likely a relatively direct reaction for nu=0, and a more intimate collision for nu=1.

*600,430*

**PB86-212941** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Observation of Interference between Quadrupole and Dipole Transitions in Low-Energy (2 eV) Photoionization from a Sodium Rydberg State.**
Final rept.,
G. Leuchs, S. J. Smith, S. N. Dixit, and P. Lambropoulos. 1986, 4p
Contract NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review Letters 56, n7 p708-711, 17 Feb 86.

Keywords: Dipoles, Atomic energy levels, Reprints, *Photoionization, *Sodium atoms, Angular distribution, Laser applications, Quadrupoles.

A measurement of the azimuthal dependence of the angular distribution of photoelectrons from 13 doublet D(3/2)-state sodium atoms aligned transversely to the direction of propagation of, and parallel to the direction of linear polarization of, 532-nm ionizing laser radiation is described. The measured distribution is 1 phi = 1 + 0.026(6)cos phi, where phi=0 is the direction of the laser beam. The departure from the symmetry 1 phi = const predicted for a pure electric dipole transition is represented theoretically as due to a dipole-quadrupole interference term.

*600,431*

**PB86-213253** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Angular Distributions of Ions Desorbing from Ti02.**
Final rept.,
R. L. Kurtz, R. Stockbauer, and T. E. Madey. 1986, 7p
Pub. in Nuclear Instruments and Methods in Physics Research B13, p518-524 1986.

Keywords: *Titanium dioxide, *Desorption, *Surface chemistry, Chemisorption, Surfaces, Ions, Reprints, Angular distribution, *Electron stimulated desorption.

The dependence of the electron- and photon-stimulated desorption (ESD, PSD) O(1+)-ion yield on surface preparation from TiO2 (110) and (001) surfaces has been studied. Angle-integrated electron-stimulated desorption yields have been measured versus annealing temperature from room temperature sputtered surfaces to 900 deg C annealed surfaces. Both the surface cation valence state and the surface geometry change as a function of annealing temperature, giving rise to a rich variety of ESD ion angular distribution (ESDIAD) patterns. These patterns are discussed in terms of possible models of local surface structure.

*600,432*
**PB86-213261** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Dynamics of Molecular Processes at Surfaces: Vibrational Lineshapes and Spectra,**
J. W. Gadzuk. 1986, 22p
Sponsored by North Atlantic Treaty Organization, Brussels (Belgium).
Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 38, p233-254 1986.

Keywords: *Surfaces, Surface chemistry, Adsorption, Vibrational spectra, Molecular spectra, Reprints.

Extremely useful connections exist between the dynamics of adsorbed molecule vibrations, as revealed in spectroscopic lineshapes, and the dynamics of molecular processes at surfaces because in both cases, the constituent atoms of a molecule, solid, or combination of the two execute multi-dimensional, motion over the same potential energy surfaces. In this paper, recent insights and advances in surface dynamics will be applied to the problem of vibrational lineshapes. Classical particle and semi-classical wavepacket dynamics will be used to address the issues of energy decay (T sub 1) vs. pure dephasing (T sub 2), overtones, and non-linear dynamics as they apply to lineshape analysis.

*600,433*
**PB86-213279** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Collision Induced Dissociation of Diatomic Molecules on Surfaces: A Charge Transfer Mechanism.**
Final rept.,
J. W. Gadzuk, and S. Holloway. 1986, 7p
Sponsored by North Atlantic Treaty Organization, Brussels (Belgium).
Pub. in Jnl. of Chemical Physics 84, n6 p3502-3508, 15 Mar 86.

Keywords: *Dissociation, Surfaces, Diatomic molecules, Excitation, Magnesium oxides, Iodine, Reprints, *Electron-molecule collisions, Molecular ions, Charge transfer.

A theory is presented which accounts for one of the possible mechanisms responsible for dissociative scattering of diatomic molecules from surfaces. If on the incident trajectory of the molecule, a surface-to-molecule electron transfer occurs and on the outgoing trajectory, the reverse, then the temporary negative molecular ion formed for the time duration between electron hops will displace in its intramolecular vibrational coordinate. The molecule will emerge as a vibrationally excited neutral, with some of the excited states lying within the dissociative continuum. A model is described for this process in which the center-of-mass translational motion is handled classically and the intramolecular motion via wave packet dynamics. The theory is energy and probability conserving and microscopically reversible. Dissociation probabilities calculated as a function of incident energy and system parameters are discussed in the light of experimental measurements for the system of I2 dissociatively scattered from MgO surfaces.

*600,434*
**PB86-213287** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Fundamental Excitations in Solids Pertinent to Desorption Induced by Electronic Transitions.**
Final rept.,
J. W. Gadzuk. 1983, 22p
Pub. in Springer Ser. Chem. Phys. 24, p4-25 1983.

Keywords: *Excitation, *Desorption, Surfaces, Chemisorption, Solids, Interactions, Reprints, Time dependence.

Various aspects of the dynamics of time-dependent localized potentials and interactions in solids and at surfaces, as they might relate to the fundamental processes involved in desorption induced by electronic transitions (DIET) are explored.

*600,435*
**PB86-213295** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Modeling the Effect of Atomic Mass Difference in Ion-Bombardment Induced Recoil Mixing of Binary Alloys,**
F. Davarya, M. L. Roush, T. D. Andreadis, and O. F. Goktepe. 1982, 5p
Pub. in Proceedings of Summer Computer Simulation Conference (1982), Denver, CO., July 19-21, 1982, p243-247.

Keywords: Computerized simulation, Mathematical models, Monte Carlo method, Surfaces, Binding energy, Atomic mass, *Ion bombardment, EVOLVE computer program, Ion implantation.

EVOLVE, a Monte Carlo computer code, is used to simulate the concentration changes which result from incident beam atoms and the cascade of recoil atoms. The changes in composition depend upon differences in the atomic masses of the target atoms, displacement energy, surface binding energy, and other factors. This study investigates the commonly held belief that lighter target elements tend to be preferentially implanted inwardly relative to heavier elements. Cases are presented here where, contrary to this perception, preferential inward movement of the heavier element was observed.

*600,436*
**PB86-214202** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**High-Resolution Infrared Spectrum of Hydrogen Peroxide the nu sub 6 Fundamental Band,**
Final rept.,
J. Hillman, D. Jennings, W. Olson, and A. Goldman. 1986, 14p
Pub. in Jnl. of Molecular Spectroscopy 117, p46-59 1986.

Keywords: *Molecular spectra, *Hydrogen peroxide, Infrared spectra, Spectroscopic analysis, Bandwidth, Reprints, High resolution, Tunable lasers, Fourier transform spectroscopy.

The infrared spectrum of the nu(sub 6) asymmetric deformation band of hydrogen peroxide (H2O2) was studied in the region 1100-1350/cm using the two techniques of Fourier transform spectroscopy at 0.02/cm resolution and tunable diode laser spectroscopy at Doppler-limited resolution. Details of the wavelength calibration procedures adopted are discussed. For the first time, accurate values of the molecular parameters of the torsionally doubled, vibrational band were obtained. A total of 708 assigned transitions have been analyzed to yield a set of 14 rovibrational constants for the lower torsion-vibration level (SD=0.00487/cm) and 13 rovibrational constants for the upper torsion-vibration level (SD = 0.00382/cm). These hybrid bands are primarily A type with band centers at 1264.5812 + or - 0.0009 and 1273.6830 + or - 0.0009/cm. Because of the absence of observed perturbations, the derived molecular constants can be used to calculate transition frequencies with a high degree of accuracy up to K(sub a) = 6.

*600,437*
**PB86-214210** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Localized Hydrogen Modes in LaNi5H(x).**
Final rept.,
R. Hempelmann, D. Richter, G. Eckold, J. J. Rush, and J. M. Rowe. 1984, 12p
Pub. in Jnl. of the Less-Common Metals 104, pl-12 1984.

Keywords: Hydrogen, Distortion, Adsorption, Vibration, Crystal lattices, Neutron scattering, Reprints, *Lanthanum nickel.

The localized vibrations of hydrogen in various LaNi5H(x) samples were studied using inelastic neutron scattering (neutron spectroscopy). The pronounced vibrational peaks obtained for 'virgin' strain-free alpha-LaNi5H0.15 indicate the existence of two different hydrogen sites. During the activation for hydrogen absorption, substantial distortion is introduced into the LaNi5 lattice which is locally probed by the vibrating hydrogen atoms.

*600,438*
**PB86-214665** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Ultraviolet Two-Photon Ionization of Molecules in Flames.**
Final rept.,
W. G. Mallard, J. Miller, and K. C. Smyth. 1985, 8p
Pub. in Lasers as Reactants and Probes in Chemistry, p127-134 1985.

Keywords: *Nitric oxides, *Phosphorous oxide, Flames, Reprints, *Multi-photon processes, Two photon absorption, Multiphoton ionization, *Photoionization.

A study was conducted on resonantly enhanced 2 photon photoionization of NO and PO in the ultraviolet region in atmospheric pressure flames. The results show that collisional refilling of the laser depopulated ground state rotational level is fast, with an effective collisional cross section > or equal to 70A. This rapid relaxation leads to photoion spectra that are essentially identical to those expected from a simple 1 photon absorption to the resonant intermediate state.

*600,439*
**PB86-214715** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Molecular X-ray Spectra: S-K(beta) Emission and K Absorption Spectra of Thiophene.**
Final rept.,
R. C. C. Perera, and R. E. LaVilla. 1986, 7p
Contract DE-AC03-76SF00098
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Chemical Physics 84, n8 p4228-4234, 15 Apr 86.

Keywords: *Thiophenes, X ray spectra, Molecular spectra, Absorption spectra, Sulfur heterocylic compounds, Reprints.

The high resolution sulfur K(Beta) emission in fluorescence and sulfur K absorption of thiophene (C4H4S) were measured with a double crystal spectrometer. The sulfur K(Beta) emission spectrum was analyzed by comparison with complementary spectral data and with MNDO and ab initio (STO-3G) MO calculations. A tentative assignment of the prominent features in the absorption spectrum was made using MO calculations as a guide. In addition the sulfur L(sub 2,3) emission spectrum was reinterpreted. The sulfur 1s binding energy of thiophene was estimated as 2477.6 eV.

*600,440*
**PB86-228673** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Photodetachment Spectroscopy of FeO(-1).**
Final rept.,
T. Andersen, K. R. Lykke, D. M. Neumark, and W. C. Lineberger. 1986, 8p
Grants NSF-CHE83-16628, NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Electronic and Atomic Collisions, p791-798 1986.

Keywords: *Iron oxides, Iron inorganic compounds, Molecular energy levels, Excitation, Molecular structure, *Photodetachment.

High-resolution autodetachment spectroscopy of FeO(1-) has been used to study the ionic ground state as well as electronically excited states located in the vicinity of the FeO(sup 5 delta sub i) thresholds. The observed autodetachment resonances suggest two qualitatively different types of electronic states in this region, a sup 4 delta valence state and two negative ion complexes consisting of an FeO(sup 5 delta sub 3) core and an s or p electron primarily bound by the dipolar electric field of the neutral core. The dependence of autodetachment lifetimes upon the rotational quantum numbers of the excited states shows markedly different properties for the two types of states. A significant difference in autodetachment lifetimes is observed for the two Lambda-doublet components assigned to the FeO-p electron complex. The authors propose that a difference in the location of the electron density of the detaching electron with respect to the plane of rotation is responsible for the Lambda-doublet effect.

*600,441*
**PB86-228970** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

**Alignment and Orientation of Atomic Outer Shells Induced by Electron and Ion Impact: Some Recent Developments and Remaining Problems.**
Final rept.,
N. Andersen, J. W. Gallagher, and I. V. Hertel. 1986, 20p
Pub. in Electronic and Atomic Collisions, p57-76 1986.

Keywords: Electron irradiation, Ion irradiation, *Electron-atom collisions, *Ion-atom collisions, *Atom-atom collisions.

Alignment and orientation of atoms in collision experiments with planar symmetry have now been studied for about 15 years and close to 500 papers have been produced, mainly devoted to S -> P excitation. Despite the large variety of electron-atom, ion-atom and atom-atom collision systems considered, a unified framework for description of these phenomena is now emerging. The framework is a generalization of the original ideas of Macek and Jaecks and is based on consideration of symmetries, conservation laws, etc. The key parameters are directly related to the shape and dynamics of the charge cloud of the excited electron as well as to experimental observables. A brief review is given of the framework, and some current problems and prospects for the future are discussed.

*600,442*
**PB86-229036** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Laser-Induced Fluctuations in Single-Photon Ionization.**
Final rept.,
K. Rzazewski. May 86, 2p
Pub. in Physical Review A 33, n5 p3527-3528 May 86.

Keywords: *Ionization, Electromagnetic noise, Band width, Variations, Reprints, Laser-produced plasma, Laser radiation.

By the example of single-photon ionization, it is shown that laser noise can induce major fluctuations of physical observables in strong-field laser-atom interactions.

*600,443*
**PB86-229044** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Mono- and Disilicon Radicals in Silane and Silane-Argon DC Discharges.**
Final rept.,
R. Robertson, and A. Gallagher. 1986, 10p
Sponsored by Solar Energy Research Inst., Golden, CO., and Department of Energy, Washington, DC.
Pub. in Jnl. of Applied Physics 59, n10 p3402-3411, 15 May 86.

Keywords: *Chemical radicals, *Silanes, Free radicals, Silicon, Surfaces, Cathodes, Electric discharges, Reprints.

Measurements of monosilicon (SiH(n)) and disilicon (Si2H(n)) radicals at the cathode surface of dc discharges in silane and silane-argon mixtures are reported. Silyl radical density per decomposed silane was constant for fixed flow conditions over a range of powers and silane-argon ratios. The relative densities for other monosilicon radicals SiH(n)/SiH3 decreased with increased fraction of silane in silane-argon mixtures. The density of disilicon radicals was observed to be comparable to some of the monosilicon radicals, with Si2H2 and Si2H4 the dominant Si2H(n) species. Formation and destruction reactions are discussed for these radicals, disilane, and the deposited film. The authors deduce that disilane is formed primarily on surfaces and that sputtering is a significant source for radicals near the cathode.

*600,444*
**PB86-229051** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Energy Transfer Processes of Aligned Excited States of Ca Atoms.**
Final rept.,
D. Neuschafer, M. O. Hale, I. V. Hertel, and S. R. Leone. 1986, 7p
Grants NSF-CHE79-11340, NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Electronic and Atomic Collisions, p585-591 1986.

Keywords: *Calcium, Orientation, Atomic orbitals, Polarization, Excitation, Energy transfer, Reprints.

Effects of orbital alignment on the near resonant energy transfer process from Ca(4s5p singlet P sub 1) to Ca(4s5p triplet P sub J) induced by collisions with rare gases are studied in a crossed molecular beam. A linearly polarized, pulsed ultraviolet laser is used to introduce the initial orbital alignment, and the relative energy transfer cross sections as a function of alignment are monitored by time-gated fluorescence detection. Different results are observed with several rare gases; a rather large, approx=50% enhancement in the rate is observed for the perpendicular vs. parallel approach with He and Ne. A smaller, but opposite effect is observed for Xe, and no effect of alignment occurs with Kr.

*600,445*
**PB86-229069** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Electron Affinities.**
Final rept.,
T. M. Miller. 1986, 4p
Pub. in CRC Handbook of Chemistry and Physics (66th Edition), pE62-E65 Aug 85-86.

Keywords: *Affinity, Negative ions.

A tabulation is provided of experimentally-determined electron affinities for 72 atoms and 197 molecules.

*600,446*
**PB86-229077** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Atomic and Molecular Polarizabilities.**
Final rept.,
T. M. Miller. 1986, 10p
Pub. in CRC Handbook of Chemistry and Physics (66th Edition), pE65-E74 Aug 85-86.

Keywords: *Polarization(Charge separation), Dielectric properties, Molecules, Atoms, *Electric dipoles.

A tabulation is provided of static electric dipole polarizabilities for 102 atoms and 366 molecules. A brief discussion is included in which the electric dipole polarizability is defined, along with the various units one encounters. A listing of formulas describing polarizability-related phenomena is given.

*600,447*
**PB86-229267** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Electron Affinities of Ge and Sn.**
Final rept.,
T. M. Miller, A. E. S. Miller, and W. C. Lineberger. 1986, 2p
Grants NSF-CHE83-16628, NSF-PHY83-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review A: General Physics 33, n5 p3558-3559 May 86.

Keywords: *Tin, *Germanium, Metals, Reprints, *Photoelectron spectroscopy, Electron affinity.

The laser photoelectron spectra of Ge(1-) and Sn(1-) are reported. Transitions in the electron detachment from the (Sup 4 S sub 3/2) ground state of the ions to the Triplet P (sub 0,1,2) states of the neutral atom are used to determine the electron affinities, 1.233 + or - 0.003 eV for Ge and 1.112 + or - 0.004 eV for Sn. The relative transition strengths to the fine-structure sublevels of the neutral do not follow the 1:3:5 statistical ratio, indicating the systematic breakdown of L-S coupling for these species.

*600,448*
**PB86-229309** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Radiatively Stabilized Collisions: Dielectronic Recombination and Radiative Association.**
Final rept.,
G. H. Dunn. 1986, 13p
Grant DOE-EA-01-A-6010
Sponsored by Department of Energy, Washington, DC.
Pub. in Electronic and Atomic Collisions, 23-36, 1986.

Keywords: *Dielectronic recombination, Ion traps, Rydberg states.

Radiatively stabilized collisions are a class to which relatively little attention has been given -- especially experimentally. In the paper two processes representative of radiatively stabilized collisions -- dielectronic recombination and radiative association -- are discussed, and recent experimental measurements on both collision types are described. Radiative association rate measurements have been carried out in a Penning ion trap at 11 K. Dielectronic recombination measurements have been made which show definitively the dependence of cross sections on extrinsic fields in the collision region and also demonstrate the dependence of cross sections on principal quantum numbers of the product Rydberg atoms.

*600,449*
**PB86-229408** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Photoabsorption Cross Section of Barium from 237.9 to 120 nm.**
Final rept.,
E. B. Saloman, J. W. Cooper, and G. Mehlman. Sep 85, 2p
Pub. in Physical Review A 32, n3 p1878-1879 Sep 85.

Keywords: *Barium, Synchrotron radiation, Far ultraviolet radiation, Near ultraviolet radiation, Reprints, *Photoabsorption.

The relative photoabsorption cross section of barium in the spectral range from the ionization limit at 237.9 to 120 nm has been measured and the results of previous measurements extending to 170 nm confirmed. The cross section is found to rise slowly at wavelengths shorter than 170 nm and to decrease in the region between 140 and 130 nm.

*600,450*
**PB86-229416** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Channel Coupling and Shape Resonance Effects in the Photoelectron Angular Distributions of the 3(sigma sub g) (-1) and 2(sigma sub u) (-1) channels of N2.**
Final rept.,
S. H. Southworth, A. C. Parr, J. E. Hardis, and J. L. Dehmer. Feb 86, 4p
Sponsored by Office of Naval Research, Arlington, VA., and Department of Energy, Washington, DC.
Pub. in Physical Review A33, n2 p1020-1023 Feb 86.

Keywords: *Nitrogen, Photoelectrons, Reprints, *Autoionization, Photoionization, Angular distribution, Channel coupling.

The authors report measurements of photoelectron angular distributions for the 3 sigma (sub g)(-1) and 2 sigma (sub u)(-1) photoionization channels of N2 from their thresholds up to 35 and 37.5 eV, respectively.

*600,451*
**PB86-229952** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Copper Spectra in a Laser-Generated Plasma: Measurements and Classifications of Cu XII to Cu XXI.**
Final rept.,
J. Sugar, and V. Kaufman. May 86, 7p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of the Optical Society of America B 3, n5 p704-710 May 86.

Keywords: Atomic energy levels, Line spectra, Reprints, *Laser-produced plasma, *Copper ions, Neodymium lasers.

A vapor containing 10- to 20-times-ionized copper was generated by focusing a 1-GW, 15-nsec, Nd-glass-laser pulse down to 0.3 mm on a metallic copper sample. Spectral radiation in the range of 125 to 450 A was recorded photographically with the National Bureau of Standards 10.7-m grazing-incidence spectrograph. Ninety-two spectral lines arising from Cu XII to Cu XXI (Ar I through F I isoelectronic sequences) were identified. Twenty-six of these, mainly in Cu XIX and Cu XXI, had been interpreted previously. Slater integrals were fitted to the energy levels derived from these data and from previously measured magnetic-dipole lines.

*600,452*
**PB86-230257** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

**Structural Studies of Passive Films Using Surface EXAFS.**
Final rept.,
J. Kruger, G. G. Long, M. Kuriyama, and A. I. Goldman. 1983, 6p
Pub. in Proceedings of International Symposium on Passivity of Metals and Semiconductors (5th), Bombannes, France, May 30-June 30, 1983, p163-168.

Keywords: *Crystal structure, *Passivity, *Films, *Surfaces, Iron, Oxides, Substrates.

Iron K-absorption edge spectra were obtained from the passive films on iron for the dried films in air (ex situ) and for the films in the passivating solutions (in situ). The ex situ results demonstrate that, while the structures of the films are more disordered than the spinel-like iron oxides (e.g. gamma -Fe2O3), they are nevertheless closely related to these crystalline oxides. The in situ data shows evidence of a quite different structure, which may be due to the accommodation of hydrogen containing species into the structure.

*600,453*
**PB86-230265** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Synchrotron Photoemission Evidence for 'Lying-Down' CO on Cr(110).**
Final rept.,
N. D. Shinn. 1986, 3p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of Vacuum Science and Technology, A4 n3 p1351-1353 May/Jun 86.

Keywords: *Carbon monoxide, *Chemisorption, *Chromium, Orientation, Molecular structure, Surfaces, Bonding, Synchrotron radiation, Ultraviolet spectroscopy, Reprints, Photoemission spectroscopy.

Synchrotron ultraviolet photoemission spectroscopy (UPS) has been used to identify two sequentially populated molecular CO binding modes on Cr(110) at 90 K. These are distinguished by both intensity and electron-binding-energy differences in the CO-derived valence-band UPS features. These results support the previously proposed models in which the first binding mode (alpha sub 1 CO) is 'lying down' on the surface, with both the carbon and oxygen coordinated to chromium atoms, and the second binding mode (alpha sub 2 CO) is terminally bonded and oriented roughly along the (110) surface normal.

*600,454*
**PB86-230273** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Calculations of Reneutralization Effects in ESDIAD (Electron Stimulated Desorption Ion Angular Distributions).**
Final rept.,
Z. Miskovic, J. Vukanic, and T. E. Madey. 1986, 9p
Pub. in Surface Science 169, p405-413 1986.

Keywords: Surfaces, Reprints, *Electron stimulated desorption, Angular distribution, Reneutralization.

Calculations are presented which describe the influence of ion reneutralization processes on measured electron stimulated desorption ion angular distributions (ESDIAD). The results indicate that reneutralization effects generally act in an opposite sense to the image field in affecting ion angular distributions, and that these counterbalancing effects tend to cancel one another partially over a wide range of polar angles.

*600,455*
**PB86-230299** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Measurements of Electron Attenuation Lengths in Condensed Molecular Solids.**
Final rept.,
R. L. Kurtz, N. Usuki, R. Stockbauer, and T. E. Madey. 1986, 24p
Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 40, p35-58 1986.

Keywords: *Methyl alcohol, *Cyclohexane, Water, Kinetic energy, Adsorption, Reprints, *Electron attenuation length, Energy range, eV range 10-100, Microcapillary array.

The attenuation lengths are approximately 13, 10 and 9A, respectively, for water, methanol and cyclohexane and show only a slight energy dependence over the electron kinetic energy range covered (18-68eV). The experiment consisted of monitoring the attenuation of Cu(100) substrate photoelectrons as solid H2O, CH3OH and C6H12 were condensed at 90 K by dosing from a microcapillary array. Accurate measurement of adsorbate layer thickness was accomplished by calibration of the doser; the procedure is described in detail.

*600,456*
**PB86-230489** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Field Effects on Rydberg Product State Distribution from Dielectronic Recombination.**
Final rept.,
G. H. Dunn, D. S. Belic, B. DePaola, N. Djuric, and D. Mueller. 1985, 16p
Contract DOE-EA-77-A-01-6010
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Workshop on Atomic Spectra and Collisions in External Fields, Gaithersburg, MD, October 22-23, 1984, Atomic Excitation and Recombination in External Fields, p405-420 1985.

Keywords: Atomic orbitals, Magnesium, *Dielectronic recombination, Rydberg states.

The effects of state mixing by extrinsic fields in the collision region have been investigated for dielectronic recombination. Using a field ionization technique, cross sections sigma sup n, sub DR have been measured as a function of the final Rydberg state, n sub f, for the dielectronic recombination process.

*600,457*
**PB86-230497** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**High-Energy Forward Elastic Scattering of Electrons: Partial-Wave Approximations.**
Final rept.,
R. K. Nesbet, and S. Geltman. Jun 86, 10p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review A 33, n6 p3815-3824 Jun 86.

Keywords: *Electron scattering, Elastic scattering, Argon, Hydrogen, Reprints, *Electron-atom collisions, Born approximation, KeV range 10-100.

Partial-wave analysis is applied to a parametrized pseudostate excitation model of high-energy electron-atom scattering. Consistency checks are carried out between asymptotic distorted-wave calculations (for coupled differential equations), second-Born-approximation scattering amplitude calculations, and partial-wave second-Born-approximation calculations. Closure formulas for partial-wave amplitude sums are derived for a static model potential and for the second-Born-approximation amplitude due to the asymptotic dipole excitation potential. Calculations using these closure formulas in e(-) + H and e(-) + Ar models at 15 keV show cusplike forward elastic scattering peaks, confirming recent exact second-Born-approximation results for an e(-) + H pseudostate model.

*600,458*
**PB86-230737** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Working Group 2: Atomic Transition Probabilities.**
Final rept.,
W. L. Wiese. 1985, 17p
Pub. in Reports on Astronomy (Transactions of the International Astronomical Union), v19A p122-138 1985.

Keywords: *Transition probabilities, *Electron transitions, *Atomic spectra, Bibliographies, Oscillator strengths.

Some new activities on the determination of atomic transition probabilities are briefly described, and an exhaustive list of new literature references is given which covers all transition probability data for the period August 1981 to the present (fall 1984).

*600,459*
**PB86-230745** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Experimental Methods for Determining Atomic Transition Probabilities.**
Final rept.,
W. L. Wiese. 1985, 25p
Pub. in Physics of Ionized Gases, p621-645 1985.

Keywords: *Transition probabilities, *Electron transitions, Oscillator strengths.

The main experimental methods for the determination of atomic transition probabilities are based on emission, absorption, and anomalous dispersion measurements. In addition, transition probabilities may also be derived from lifetime determinations of excited atomic states. All these approaches have undergone significant modifications and refinements in recent years, and some new experimental tools and combinations of techniques have been added. As a result, impressive accuracies have been reached and the ranges of applicability of some approaches have been greatly enlarged. These advances and developments, as well as remaining problem areas, will be described and illustrated with a number of typical examples.

*600,460*
**PB86-230760** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Comprehensive, Consistent Thermodynamic Tables.**
Final rept.,
D. Garvin, and H. J. White. 1986, 112p
Pub. in Committee on Data for Science and Technology Bulletin No. 58, Chapter 1, p1-112 1986.

Keywords: *Thermodynamics, Tables(Data).

No abstract available.

*600,461*
**PB86-230778** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Discrimination of C3H3+ Structures on the Basis of Chemical Reactivity.**
Final rept.,
P. Ausloos, and S. G. Lias. 1981, 3p
Pub. in Jnl. of American Chemical Society 103, n21 p6505-6507 1981.

Keywords: *Chemical reactivity, Reaction kinetics, Flames, Acetylene, Molecular structure, Benzene, Reprints, *Cyclopropenium ions, *Ion-molecule collisions, Ion cyclotron resonance spectroscopy, Molecular ions.

Kinetic evidence is presented for the existence of C3H3(1+) ions in two distinct isomeric structures, cyclo-C3H3(1+) and C3H2(1+), when these ions are produced through the decomposition of a variety of molecular ions. The relative abundance of the two isomeric C3H3(1+) ions depends on the identity of the precursor molecule as well as the internal energy of the dissociating parent ion. While the cyclo-C3H3(1+) ions do not react with acetylene, C3H3(1+) ions react to give C5H5(1+) and C5H3(1+) products; these ions, and the products of their further reactions are seen in acetylene flames, and have been suggested to be the precursors in the mechanism leading to soot formation. Reactions of the two C3H3(1+) ions with benzene, olefins, and other compounds are discussed.

*600,462*
**PB86-230935** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Universal Amplitude Ratios and the Interfacial Tension Near Consolute Points of Binary Liquid Mixtures.**
Final rept.,
H. Chaar, M. R. Moldover, and J. W. Schmidt. 1986, 10p
Pub. in Jnl. of Chemical Physics 85, n1 p418-427, 1 Jul 86.

Keywords: *Cyclohexane, *Methyl alcohol, Density, Heavy water, Tertiary amines, Liquids, Reprints, Binary systems(Materials), *Interfacial tension, Binary mixtures, Thermophysical properties, Amplitude ratios.

The densities of the coexisting phases and the capillary length have been measured to obtain the interfacial tension (sigma) near the consolute temperatures T sub c of the three binary liquid mixtures: triethylamine

+ water, triethylamine + heavy water, and methanol + cyclohexane.

*600,463*
**PB86-231131** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Spin-Dependent Superelastic Scattering from Pure Angular Momentum States of Na(3P).**
Final rept.,
J. J. McClelland, M. H. Kelley, and R. J. Celotta. 1986, 4p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review Letters 56, n13 p1362-1365, 31 Mar 86.

Keywords: Atomic energy levels, Electron scattering, Excitation, Elastic scattering, Reprints, *Electron-atom collisions, *Sodium atoms, Electron spin polarization.

Spin asymmetries are presented for superelastic scattering of spin-polarized electrons from spin-polarized M sub L = + 1 and M sub L = - 1 states of the Na 3P(3/2) atom. The incident-energy dependence at a scattering angle of 30 deg is shown for energies of 1.26 to 11.76 eV. In addition, angular dependences over the range 5 deg to 40 deg are given at 2.0 and 9.26 eV. Large differences are seen between the spin asymmetries for the two M sub L sublevels of the excited state, with the M sub L = - 1 asymmetry reaching a value of 100% at 2 eV and 35 deg scattering angle, corresponding to pure singlet scattering.

*600,464*
**PB86-231149** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Far Infrared Spectrum of Magnesium Hydride.**
Final rept.,
K. R. Leopold, L. R. Zink, K. M. Evenson, D. A. Jennings, and M. Mizushima. 1986, 3p
Pub. in Jnl. of Chemical Physics 84, n3 p1935-1937, 1 Feb 86.

Keywords: *Interstellar matter, *Magnesium hydrides, *Infrared spectra, Atomic energy levels, Ground state, Rotational spectra, Far infrared radiation, Reprints.

The rotational spectrum of MgH in its ground doublet Sigma has been observed for the first time using a new tunable far infrared spectrometer. The molecular constants derived are of sufficient accuracy to permit astrophysical identification of the species.

*600,465*
**PB86-231552** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Sub-Doppler Infrared Absorption Spectroscopy of Ar-HF ((10 sup 0) <- (00 sup 0)) in a Linear Supersonic Jet.**
Final rept.,
C. M. Lovejoy, M. D. Schuder, and D. J. Nesbitt. 20 Jun 86, 3p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Chemical Physics Letters 127, n4 p374-376, 20 Jun 86.

Keywords: *Argon, *Hydrogen fluoride, Absorption, Infrared spectroscopy, Reprints, Tunable lasers.

Ultra-sensitive tunable difference frequency IR absorption spectroscopy in a slit supersonic jet has been used to observe sub-Doppler spectra of Ar-HF in the (10 sup 0 0) HF stretch and (11 sup 1 0) HF stretch plus van der Waals bend modes. Linewidths yield a lower limit of 3 x 10 to the -9th power s for the predissociation lifetime in the vibrationally metastable upper state. The sensitivity of these direct absorption methods (< or approx. equal to 2 x 10 to the 9th power molecules/cc per quantum state), in conjunction with the wide tunability of the difference frequency laser (2.2-4.2 micrometers permit high-resolution studies of a large class of van der Waals complexes.

*600,466*
**PB86-232345** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Rotational Spectrum and Structure of CF3H-NH3.**
Final rept.,
G. T. Fraser, F. J. Lovas, R. D. Suenram, D. D. Nelson, and W. Klemperer. 1986, 6p
Pub. in Jnl. of Chemical Physics 84, n11 p5983-5988, 1 Jun 86.

Keywords: *Molecular structure, *Ammonia, Rotational spectra, Excitation, Reprints, *Methane/trifluoro.

The rotational spectrum of CF3H-NH3 has been obtained using a pulsed nozzle Fourier transform microwave spectrometer. A symmetric top spectrum is observed that is consistent with free internal rotation of the NH3 subunit against the CF3H subunit. Rotational transitions have been measured for both the ground and first excited internal rotor state of the complex. The spectroscopic constants which have been obtained include: B sub 0=1996.903(2) MHz, D sub J=3.46(12) kHz, and eQ(q sub N) = -3.186(8) MHz. From the quadrupole coupling constant of the nitrogen nucleus, eQ(q sub N), the bending amplitude of the NH3 unit is determined to be 22.57(10) deg. The hydrogen bond length is 2.314(5) A and the weak bond stretching force constant is 0.066(2) mdyn/A. The bond length and stretching force constant for CF3H-NH3 are similar in value to those determined for HCCH-NH3 (2.33 A and 0.070 mdyn/A, respectively).

*600,467*
**PB86-232733** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Line Interference Effects in the Vibrational Q-Branch Spectra of N2 and CO.**
Final rept.,
G. J. Rosasco, W. Lempert, W. S. Hurst, and A. Fein. 1983, 6p
Pub. in Chemical Physics Letters 97, n4/5 p435-440, 27 May 83.

Keywords: *Nitrogen, *Raman spectra, *Carbon monoxide, Ramon spectroscopy, Reprints.

Self-broadened (about 20-200 kPa) Q-branch spectra are measured by high resolution CW stimulated Raman spectroscopy. Line overlap in these spectra is described in a relaxation matrix formalism and a first order (in density) solution to the resulting equation is used to fit the data. The parameters of the model are analyzed in terms of rates of rotational energy transfer.

*600,468*
**PB86-232741** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Phase Space Subdivision of the Second Virial Coefficient.**
Final rept.,
D. G. Friend. 1985, 5p
Sponsored by National Research Council, Washington, DC.
Pub. in Jnl. of Chemical Physics 82, n2 p967-971, 15 Jan 85.

Keywords: Reprints, *Virial coefficients, Phase space, Metastable states.

The division of two-body relative space into free, bound, and metastable subspaces is presented in terms of fundamental variables. This enables us to examine the differences among the various partitions of the second virial coefficient presented by Rainwater, as boundary effects. Explicit evaluations of these boundary contributions are presented in certain cases and agreement is obtained between this and the earlier approach to the problem. For the bound subspace, in particular, an identity is established which relates the partition function and potential formulations of the second virial coefficient.

*600,469*
**PB86-232964** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Laser Desorption Mass Spectrometry of Squaric Acid and Its Salts.**
Final rept.,
G. D. Byrd, A. J. Fatiadi, D. S. Simons, and E. White. 1986, 6p
Pub. in Organic Mass Spectrometry 21, p63-68 1986.

Keywords: *Desorption, Mass spectroscopy, Reprints, *Cyclobutene-dione/dihydroxy.

The laser desorption mass spectrometry of the oxocarbon squaric acid (3,4-dihydroxy-3-cyclobutene-1,2-dione) and its salts of the form A2C4O4 (A=cation) is described. Both positive and negative ion spectra were obtained. The positive ion spectrum of the acid is characterized by an ion corresponding to loss of CO from (M+H)(1+). The negative ion spectrum shows an intense (M-H) (1-) peak in addition to a dimer species. The alkali salt spectra contain (M+A) (1+) in the positive mode and (M-A)(1-) and an intense (C4HO4) (1-) in the negative mode. The smaller alkali salts also have an (M+H) (1+) adduct ion. Unlike the alkali squarates, the ammonium salt shows ions corresponding to losses of neutrals from the molecular adduct in the positive ion spectrum and a dimer species in the negative ion spectrum. Molecular weight information was obtained in all cases. A (bis)dicyanomethylene derivative of potassium squarate was also studied. Some field desorption mass spectrometry results are presented for comparison.

*600,470*
**PB86-235827** PC **A99/MF E04**
National Bureau of Standards, Boulder, CO.
**Proceedings of the International Symposium on Free Radicals (17th) Held at Granby, Colorado on August 18-23, 1985,**
K. M. Evenson. Apr 86, 787p NBS/SP-716
Also available from Supt. of Docs. as SN003-003-02742-1. Sponsored by Spectra Physics, Inc., Bedford, MA. Laser Analytics Div., National Aeronautics and Space Administration, Washington, DC., Smithsonian Astrophysical Observatory, Cambridge, MA., and Oriel Corp., Stratford, CT.

Keywords: *Free radicals, *Meetings, Chemical radicals, Low temperature research, Chemical reactions, Reaction kinetics, Complex compounds, Spectroscopy, Photodissociation.

The publication contains a total of 67 papers which appears in written form. Partial listing includes: Difference frequency laser spectroscopy of polyatomic ions; Kinetics of hydroxyl radical reactions with alkyl radicals; Vibration rotation spectroscopy of open-shell molecular ions; Faraday-LMR of DC(1+) in a DC-Discharge; The low-temperature measurements of the 'dimol' emission from singlet molecular oxygen; Laser spectroscopy of organometallic free radicals; Fourier transform detection of laser induced fluorescence from CCN and SrOH; Atmospheric free radicals: detection, calibration, and field measurement; Some studies of the atmospheric reactions of NO3 and FTIR matrix isolation spectrum of NO3; The far-infrared LMR spectrum of the CN radical; Inner and outer nitrogen hyperfine structure in the HN2(1+) molecular ion; Far-infrared measurements of stratospheric trace gases; Multiphoton ionization studies of UV-multiphoton fragmentation processes.

*600,471*
**PB86-238300** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Rovibrational Analysis of an Intermolecular Hydrogen-Bonded Vibration: The nu(sub 6, sup 1) Band of HCN---HF.**
Final rept.,
B. A. Wofford, M. W. Jackson, J. W. Bevan, W. B. Olson, and W. J. Lafferty. 1986, 4p
Grant NSF-CHE83-00592
Sponsored by National Science Foundation, Washington, DC., and Robert A. Welch Foundation, Houston, TX.
Pub. in Jnl. of Chemical Physics 84, n11 p6115-6118, 1 Jun 86.

Keywords: *Infrared spectra, *Hydrogen cyanide, *Hydrogen fluoride, Hydrogen bonds, Molecular vibration, Reprints.

The infrared spectrum of the intermolecular bending vibration, the nu(sub 6, sup 1) band, of the heterodimer HCN-HF has been obtained with 0.010/cm resolution, and the rotational structure of the band has been assigned. The spectroscopic constants of the nu(sub 6, sup 1) state in cm are: Nu sub 0 = 550.0285(2); B sub 6 = 0.117652 9(10); D(sub J, sup 6) = 0.2791(5) x 10 to the -6 power; q sub 6= 0.579(8)x10-4; alpha sub 6= -0.002137(1), where the uncertainties cited are one standard deviation.

*600,472*
**PB86-238672** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

**Energy and Radiative Lifetime of the 5d(9) 6s(2) doublet D(5/2) State in Hg II by Doppler-Free Two-Photon Laser Spectroscopy.**
Final rept.,
J. C. Bergquist, D. J. Wineland, W. M. Itano, H. Hemmati, and H. U. Daniel. 7 Oct 85, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Physical Review Letters 35, n15 p1567-1570, October 7, 1985.

Keywords: Atomic orbitals, Reprints, *Electronic structure, *Mercury ions.

The Doppler-free, two-photon 5d10 6s doublet S sub 1/2 - 5d9 6s22 D sub 5/2 transition in singly ionized Hg, attractive as an optical-frequency standard, has been observed for the first time on a small number of (198)Hg(1+) ions confined in a radio-frequency trap. The radiative lifetime of the doublet D sub 5/2 state and the absolute wave number of the two-photon transition were measured to be 0.090(15) s and 17757.152(3)/cm, respectively. Optical amplitude-modulation sidebands, induced by the secular (thermal) motion of the harmonically bound ions, were observed also for the first time.

*600,473*
**PB86-238912** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Rotational Analysis and Vibrational Predissociation in the (nu sub 2) Band of HCN Dimer.**
Final rept.,
B. A Wofford, J. W. Bevan, W. B. Olson, and W. J. Lafferty. 1 Jul 86, 4p
Grant NSF-CHE83-00592
Sponsored by National Science Foundation, Washington, DC., and Robert A. Welch Foundation, Houston, TX.
Pub. in Jnl. of Chemical Physics 85, n1 p105-108, 1 Jul 86.

Keywords: *Hydrogen cyanide, *Molecular structure, Vibrational spectra, Rotational spectra, Infrared spectra, Excitation, Hydrogen bonds, Reprints.

The rovibrational infrared spectrum of the bound C-H stretching vibration, nu(sub 2), in the HCN dimer has been analyzed. Observed transition frequencies have been combined with previously recorded microwave data to obtain the following molecular parameters (in cm): nu(sub 2)= 3241.5696(8), alpha(sub 2)=-0.000 110(1), B(double prime) = 0.058 233 92(1), B(sup prime)=0.058 344(1), (D(sub J), double prime)= 0.7013(52) x 10 to the -7th power, D'J=0.6636(18) x 10 to the -7th power. The observed full widths at half-maximum intensity of the observed transitions are consistent with excited state lifetimes of 1.7(4) x 10 to the -9th powers.

*600,474*
**PB86-239084** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Local Exchange Approximations.**
Final rept.,
A. W. Weiss. Jul 86, 2p
Pub. in Physical Review A 34, n1 p624-625 Jul 86.

Keywords: Wave functions, Approximation, Reprints, *Exchange interactions, Hartree-Fock method.

It is shown for the particular example of a berylliumlike atom that the Hartree-Fock 2s inflection point does not occur at the node of the wave function, as it must for a central potential. Local exchange approximations, therefore, cannot be expected to be capable of exactly modeling the effect of the exchange interaction.

*600,475*
**PB86-239092** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Accurate Energies for the Low-Lying Levels of Singly Ionized (198)Hg.**
Final rept.,
J. Reader, and C. J. Sansonetti. Feb 86, 4p
Pub. in Physical Review A 33, n2 p1440-1443 Feb 86.

Keywords: Atomic energy levels, Atomic orbitals, Wavelengths, Ionization, Reprints, *Mercury ions, *Electronic structure, *Mercury 198.

A 3.34-m plane-grating spectrograph has been used to measure the wavelengths of 11 lines of singly ionized (198)Hg emitted by an electrodeless discharge lamp in the region 1942-7944. The uncertainty varies from + or -0.0003 to + or -0.0015. From these wavelengths, accurate values were determined for all levels of the 5d10 6s, 6p, 6d, 7s, 7p, and 5d9 6s2 configurations and for four levels of the 5d9 6s 6p configuration. By using existing isotope-shift data, values of wavelengths and energy levels for natural Hg II were deduced. Accurate values for 12 lines of Hg II in the region 893-2026 were calculated from the energy levels.

*600,476*
**PB86-239100** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**4s(2) singlet S(sub 0) - 4s4p singlet P(1) Transitions in Zinclike Ions.**
Final rept.,
N. Acquista, and J. Reader. 1984, 3p
Sponsored by Department of Energy, Washington, DC. Office of Magnetic Fusion Energy.
Pub. in Jnl. of the Optical Society of America B-Optical Physics 1, n4 p649-651 1984.

Keywords: Atomic orbitals, Iron, Ultraviolet spectra, Reprints, *Isoelectronic sequence, *Electronic structure, Laser-produced plasma.

The 4s2 singlet S sub 0 - 4s 4p singlet P sub 1 transitions of twenty zinclike ions from Ru(14+) to Dy(36+) were observed with a laser-produced plasma and a 10.7-m grazing-incidence spectrograph. Also, new observations were made for the 3d-4f transitions of Fe(15+). Based on the new wavelengths obtained for these Fe transitions and improved wavelengths recently published for other Fe ions, revised values were determined for the 4s2 singlet S sub 0 - 4s 4p singlet P sub 1 transitions in ten zinclike ions from Ba(26+) to W(44+) observed by Reader and Luther, where a laser-produced spectrum of Fe was used for wavelength calibration.

*600,477*
**PB86-239282** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Simplified Method for Calculating Four-Probe Resistances on Nonuniform Structures.**
Final rept.,
H. L. Berkowitz, and J. Albers. 1984, 1p
Pub. in Electrochemical Society Extended Abstracts 84-2, p751 1984.

Keywords: *Electrochemistry, Four probe resistance, Numerical solution.

A simple method for calculating the four-probe resistance as an integral involving only the kernel of the correction factor integral (and independent of the probe radius and the probe-current density) is presented. Analytic expressions are derived for uniform layers and are investigated as a function of the probe spacing. For nonuniform resistivity structures, a simple numerical procedure is presented for the evaluation of the four-probe resistance and is compared with more extensive techniques.

*600,478*
**PB86-239720** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Rovibrational Analysis of (nu sub 3) HCN---HF Using Fourier Transform Infrared Spectroscopy.**
Final rept.,
B. A. Wofford, J. W. Bevan, W. B. Olson, and W. J. Lafferty. 15 Dec 85, 5p
Grant NSF-CHE83-00592
Sponsored by National Science Foundation, Washington, DC., and Robert A. Welch Foundation, Houston, TX.
Pub. in Jnl. of Chemical Physics 83, n12 p6188-6192, 15 Dec 85.

Keywords: *Molecular structure, *Hydrogen cyanide, *Hydrogen fluoride, Vibrational spectra, Rotational spectra, Infrared spectroscopy, Excitation, Reprints, Fourier transform spectroscopy.

The gas phase rovibrational spectrum of the (nu sub 3) band arising from the cyanide stretching vibration in the hydrogen bonded heterodimer HCN---HF has been observed at 0.004/cm instrumental resolution using a Fourier transform infrared spectrophotometer. Analysis of the spectrum gave the following molecular parameter (in/cm): (nu sub 3)=2120.935(12), (alpha sub 3)= + 5.06(19) x 10 to the -4 power, B'= 0.119 283(19), (D sub j)= 2.30(7) x 10 to the -7 power. Excited state amplitude lifetimes of observed transitions are demonstrated to be 5.6(4) x 10 to the -10 power s.

*600,479*
**PB86-239738** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Determination of A (sub 0) for CH3D from Perturbation-Allowed Transitions.**
Final rept.,
C. Chackerian, E. S. Bus, W. B. Olson, and G. Guelachvili. 1986, 6p
Pub. in Jnl. of Molecular Spectroscopy 117, p355-360 1986.

Keywords: *Molecular structure, *Methane, Ground state, Infrared spectroscopy, Deuterium compounds, Reprints.

Ground state combination differences obtained from normally allowed and perturbation-allowed transitions in the 2 nu (sub 6) band of (12) CH3D have been fitted to obtain the following values for rotational constants: A (sub 0)=5.2508231 + or - 0.0000043/cm, and D sub 0, sup K)=(-7.869 + or -0.23) x 10 to the -5th power/cm.

*600,480*
**PB86-240462** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Final-State Distribution for Na(3P sub J) + Na(3P sub J prime) > Na(nL sub J double prime) + Na(3S sub 1/2) Collisional Excitation Transfer.**
Final rept.,
S. A. Davidson, J. F. Kelly, and A. Gallagher. 1986, 11p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physical Review A: General Physics 33, n6 p3756-3766 Jun 86.

Keywords: *Sodium, *Excitation, Energy transfer, Reprints, *Molecule-molecule collisions, *Electronic state.

The authors report the ratio of rate coefficients for the excitation-transfer reaction Na(3P(sub J)) + Na(3P(sub J)) -> Na(nL(sub J double)) + Na(3S (sub 1/2)), which has sometimes been labeled energy pooling, measured in a cell at T=640 K. Rate-coefficient ratios are given for nL(sub J double prime = 4D (sub 3/2), 4D (sub 5/2), 4F(sub 5/2), 4F(sub 7/2), and 5S(sub 1/2), each for J= J'= 1/2 and 3/2. The authors also report the (nL(sub J double prime)) ratios when the 3P states are populated in nearly statistical ratios; these are related to the rate coefficients when J=1/2 and J'3/2.

*600,481*
**PB86-240488** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Characterization of OH(ad) Formation by Reaction between H2O and O(ad) on Ag(110).**
Final rept.,
K. Bange, T. E. Madey, and J. K. Sass. 1985, 9p
Pub. in Surface Science 152, p550-558 Apr 85.

Keywords: *Oxygen, *Water, *Silver, *Surface chemistry, Chemical reactions, Reprints, *Hydroxyl radicals.

TDS (thermal desorption spectroscopy), LEED (low energy electron diffraction) and ESDIAD (electron stimulated desorption ion angular distribution) have been used to characterize hydroxyl groups formed by the reaction of oxygen and water on Ag(110). It is concluded that hydroxyl formation on Ag(110) is accompanied by large translation of O(ad) and OH9ad) along troughs and across ridges.

*600,482*
**PB86-240769** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

**Measurements of the g(sub J) Factors of the 6s doublet S(1/2) and 6p doublet P(1/2) states in (198)Hg(1+).**
Final rept.,
W. M. Itano, J. C. Bergquist, and D. J. Wineland. Sep 85, 3p
Pub. in Jnl. of the Optical Society of America B 2, n9 p1392-1394 Sep 85.

Keywords: Magnetic moments, Resonance absorption, Atomic spectroscopy, Reprints, *Mercury ions, *Electronic structure, *Mercury 198, Ion storage.

Measurements of (198)Hg(1+) g sub J factors by two methods are reported. The first method was based on optical wavelength measurements of the Zeeman components of the 6s doublet S sub 1/2 (ground state) to 6p doublet P sub 1/2 transition at 194 nm. The lines were observed by the absorption of tunable 194-nm radiation by Hg(1+) ions created in a rf discharge. The results were g sub J (6s doublet S 1/2) = 2.0036(20) and g sub J (6p doublet S 1/2) = 0.6652(20). The second method was based on microwave-optical double resonance of ions confined in a Penning trap. They were optically pumped by the 194-nm source, which was tuned to a particular Zeeman component. An increase in the resonance-fluorescence intensity was observed when the microwave frequency was tuned to the ground-state Zeeman resonance. The result is g sub J (6s doublet S 1/2) = 2.003 174 5*74).

*600,483*

**PB87-100228**
(Order as PB87-100186, PC **A08**/MF **A01**)
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Thermophysical Property Measurement on Chemically Reacting Systems: A Case Study,**
T. J. Bruno, and G. C. Straty. Jun 86, 4p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Included in Jnl. of Research of the National Bureau of Standards, v91 n3 p135-138 May-Jun 86.

Keywords: *Chemical reactions, *Carbinals, Thermophysical properties, Decomposition, Methyl alcohol, High temperature.

Thin short paper describes several experimental approaches for dealing with chemical reactions or decomposition which can occur when making thermophysical property measurements at high temperature and high pressure. The associated equipment was designed and built to allow thermophysical property data to be cast in a more realistic perspective by taking explicit account of chemical changes which may occur during an experiment. As an example of these methods, the measurements on the methanol system are discussed in detail.

*600,484*

**PB87-103255** PC **A06**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Thermodynamic Properties of Nitrogen Tetroxide.**
Final rept.,
R. D. McCarty, H. U. Steurer, and C. M. Daily. Jul 86, 106p NBSIR-86/3054
Contract NASA-CC-26848B
Sponsored by National Aeronautics and Space Administration, Cocoa Beach, FL. John F. Kennedy Space Center.

Keywords: *Chemical equilibrium, Thermodynamic properties, Mathematical models, Equations of state, Temperature, Density, Tables(Data), Chemical composition, *Nitrogen tetroxide.

A mathematical model of the equation of state of nitrogen tetroxide is presented. Isobaric tables of P-rho-T and composition for temperatures from the triple point (261.95 K) to 600 K with pressures to 40 MPa are also given. The mathematical model of the equation of state is a 32 term modified Benedict-Webb-Rubin equation. A method of calculating chemical equilibrium for the system is also presented.

*600,485*

**PB87-104022** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Quasi-Penning Resonances of a Rydberg Electron in Crossed Electric and Magnetic Fields.**
Final rept.,
C. W. Clark, E. Korevaar, and M. Littman. 1985, 3p
Pub. in Physical Review Letters 54, n4 p320-322, 28 Jan 85.

Keywords: Electrons, Electric fields, Magnetic fields, Resonance, Reprints, *Rydberg states, Penning traps.

It is shown that the combination of crossed electric and magnetic fields and the Coulomb field of the atomic nucleus can lead to the localization of the Rydberg electron in the vicinity of the Stark saddle point. The localization principle is shown to be similar to the one which serves as the basis for a Penning trap. The localized electron is expected to give rise to quasi-bound states near and above the saddle-point ionization limit. These states are expected to cause modulations in the threshold photoionization cross sections.

*600,486*

**PB87-104030** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Isotope Shifts of Some Ultraviolet Transitions of First Row Elements.**
Final rept.,
C. W. Clark. 1984, 3p
Contract DE-AI05-83ER60185
Sponsored by Department of Energy, Washington, DC.
Pub. in Astrophysical Jnl 285, n1 p322-324, 1 Oct 84.

Keywords: *Isotope effect, *Alkali metal compounds, *Interstellar matter, Ultraviolet radiation, Reprints, Atomic interactions.

Attention is drawn to the existence of unusually large isotope shifts in the spectra of first row elements, and a simple explanation for the phenomenon is given. Calculated values of these shifts are presented, which are believed accurate to within 10-20%; they agree well with the available experimental data, which is very sparse, and with other theoretical values. Some of these shifts could be employed for isotopic abundance studies of interstellar matter, when sufficient resolution in the ultraviolet range becomes available.

*600,487*

**PB87-104048** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Enhancement of the Isotopic Abundance Sensitivity of Mass Spectrometry by Doppler-Free Resonance Ionization.**
Final rept.,
C. W. Clark, J. D. Fassett, T. B. Lucatorto, and L. J. Moore. 1984, 11p
Contract DE-AI05-83ER60185
Sponsored by Department of Energy, Washington, DC.
Pub. in Resonance Ionization Spectroscopy 1984, p107-117.

Keywords: Excitation, Mass spectroscopy, Sensitivity, Ionization, Geochronology, Reprints, *Resonance ionization mass spectrometry, *Carbon atoms, Isotope dating.

The use of two-photon Doppler-free excitation in atomic resonance ionization offers the possibility of considerable enhancement of the isotopic abundance sensitivity of conventional mass spectrometry. In some applications of interest, e.g. carbon dating, this technique may provide sensitivity comparable to that presently attained by accelerator-based high energy mass spectrometry. The authors discuss the basic physics underlying the method, and describe preliminary experimental work on three-photon ionization of atomic carbon.

*600,488*

**PB87-104063** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Adiabatic Hyperspherical Treatment of Lithium doublet P States.**
Final rept.,
C. H. Greene, and C. W. Clark. 1984, 9p
Pub. in Physical Review A: General Physics 30, n5 p2161-2169 Nov 84.

Keywords: *Atomic structure, Excitation, Atomic energy levels, Reprints, *Lithium atoms, Autoionization, Hyperspherical coordinate method.

The lithium atom is studied by treating all three electrons on an equal footing using hyperspherical coordinates. The use of asymptotic base states improves the convergence of the potential curve calculation dramatically at large R. A potential curve plot suggests that a few localized pathways dominate the formation and decay of the lowest triply-excited state, 2s2 2p. A quantitative study of the lowest state of the symmetry, 1s2 2p, shows that the adiabatic approximation in hyperspherical coordinates gives an improvement over independent-electron methods, owing primarily to its inclusion of radial correlation effects at small distances R.

*600,489*

**PB87-104089** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Doppler-Free Two-Photon Laser Spectroscopy of HgII.**
Final rept.,
J. C. Bergquist, D. J. Wineland, W. M. Itano, H. Hemmati, and H. U. Daniel. 1986, 3p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Proceedings of Annual Symposium on Frequency Control (39th), Philadelphia, PA., May 29-31, 1985, p85-87.

Keywords: *Atomic orbitals, Doppler effect, Atomic energy levels, Frequency standards, Reprints, *Mercury ions, *Mercury 198, Ion traps, Laser cooling, Two photon adsorption.

The Doppler-free, two-photon 5d10 6s2 doublet S(sub 1/2) - 5d9 6s2 doublet D (sub 5/2) transition in singly ionized Hg, attractive as an optical frequency standard, has been observed for the first time. A few 198 Hg(1+) ions were confined in a radio-frequency (rf) trap and the two-photon transition was detected by monitoring the change in the fluorescence light scattered by the ions from a laser beam tuned to the first resonance transition at 194 nm. The radiative lifetime of the doublet D sub 5/2 state and the absolute wavenumber of the two-photon transition were measured to be 0.090(15) s and 17 757.152(3) /cm respectively.

*600,490*

**PB87-104097** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Laser-Magnetic-Resonance Detection of Magnesium Atoms in the Metastable triplet P (sub 0,1,2) States.**
Final rept.,
M. Inguscio, K. R. Leopold, J. S. Murray, and K. M. Evenson. 1985, 4p
Grant NASW-15 047
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of the Optical Society of America B2, n9 p1566-1569 Sep 85.

Keywords: *Metastable state, Far infrared radiation, Atomic structure, Reprints, *Magnesium atoms, Laser magnetic resonance, Fine structure, G factor.

Transitions between fine-structure levels of the metastable (3s3p triplet P) state of magnesium have been observed by means of the highly sensitive technique of far-infrared laser-magnetic-resonance spectroscopy. The g factors for the triplet P sub 1 and triplet P sub 2 levels are 1.50111(16) and 1.50102(16), respectively, and the triplet P(sub 1) - triplet P(sub2) energy separation is 1 220 575.1(33) MHz. The observed g factors show good agreement with the predicted values. This stands in marked contrast to similar results for atomic silicon (triplet P) and aluminum (doublet P), for which the theoretical and experimental g factors differ substantially. The value of the triplet P(sub 1) - triplet P(sub 2) energy separation is improved by nearly 2 orders of magnitude over the optical value and is of sufficient accuracy to permit possible extraterrestrial identification.

*600,491*

**PB87-104105** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

**Far Infrared Laser Magnetic Resonance of Metastable (triplet P) Mg.**
Final rept.,
M. Inguscio, K. R. Leopold, J. M. Murray, and K. M. Evenson. 1984, 2p
Pub. in Proceedings of International Conference on Infrared and Millimeter Waves (9th), Takarazuka (Japan), 22-26 October 1984, p96-97.

Keywords: *Magnesium, Far infrared radiation, Zeeman effect, Metastable state, Reprints, Gyromagnetic ratio, Laser magnetic resonance, Fine structure.

Laser Magnetic Resonance spectroscopy inside the cavity of an optically pumped Fir laser has been successfully extended to the detection of a refractory atom in metastable states. Several coincidences with frequency measured laser lines are detected both for the 0 - 1 and 1 - 2 transitions of the metastable triplet P(sub 0,1,2) state of Mg. The fine structure separation is determined as well as the gyromagnetic factors.

*600,492*
**PB87-104253** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Shear Viscosity Coefficients of Compressed Gaseous and Liquid Carbon Dioxide at Temperatures between 220 and 320 K and at Pressures to 30 MPa.**
Final rept.,
D. E. Diller, and M. J. Ball. 1985, 11p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in International Jnl. of Thermophysics 6, n6 p619-629 Nov 85.

Keywords: *Carbon dioxide, *Viscosity, Thermophysical properties, Density(Mass/volume), Temperature, Reprints, High pressure.

The shear viscosity coefficients of compressed gaseous and liquid carbon dioxide have been measured with the torsional piezoelectric crystal method at temperatures between 220 and 320 K and at pressures to 30 MPa. The dependencies of the viscosity on pressure, density, and temperature and the dependencies of the fluidity (inverse viscosity) on molar volume and temperature have been examined. The measurements on the compressed liquid were correlated with a modified Hildebrand equation.

*600,493*
**PB87-104451** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Anomalous Pressure-Dependence of the Torsional Levels in Solid Nitromethane.**
Final rept.,
D. Cavagnat, A. Magerl, C. Vettier, I. Anderson, and S. F. Trevino. 1985, 4p
Pub. in Physical Review Letters 54, n3 p193-196 1985.

Keywords: Neutron scattering, Molecular structure, Inelastic scattering, Reprints, *Methane/nitro, Pressure dependence.

Inelastic neutron scattering measurements of the torsional levels of CH3NO2 and CD3NO2 are presented as functions of pressure and temperature. In contrast to all previously observed pressure dependence of hindered rotors, the ground state tunnel splitting increases and the energy of the bound torsional levels decrease with pressure. A potential which reproduces these anomalous effects is found and the source of the anomanly explained.

*600,494*
**PB87-105045** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.
**Simple Model for Coherent Equilibrium.**
Final rept.,
J. W. Cahn, and F. Larche. 1984, 9p
Pub. in Acta Metallurgica 32, n11 p1915-1923 1984.

Keywords: *Phase diagrams, Thermodynamics, Elastic properties, Reprints, Coherence.

The authors prove by a simple counterexample that many general theorems of fluid phase equilibrium are not valid for coherent phase equilibrium. Many discrepancies among solid state phase diagram determinations could be the result of applying thermodynamic theorems, whose proofs are invalidated by the presence of an elastic energy term in the free energy.

*600,495*
**PB87-105169** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Improved Mixing Rules for One-Fluid Conformal Solution Calculations.**
Final rept.,
J. F. Ely. 1986, 20p
Pub. in Equations of State: Theories and Applications, ch. 16 p331-350 1986.

Keywords: *Fluids, Equations of state, Thermodynamics, Leonard-Jones potential, Mean density approximation.

During the past few years there has been great interest in improving equation of state mixing rules for fluid modeling. In the report new one-fluid mixing rules are proposed which explicitly take size difference effects into account. The resulting rules give the hard sphere mixture compressibility factor exactly. Comparisons of predicted excess properties for Lennard-Jones mixtures of varying size and energy ratios are presented. The results of the new mixing rules are superior to the van der Waals one-fluid model, especially for the excess volume.

*600,496*
**PB87-105805** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Microwave and Far-Infrared Spectra of the (sup 18)OH Radical.**
Final rept.,
E. R. Comben, J. M. Brown, T. C. Steimle, K. R. Leopold, and K. M. Evenson. 1986, 5p
Grant NASW-15047
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 305, p513-517, 1 Jun 86.

Keywords: Infrared spectra, Chemical radicals, Microwave spectra, Rotational spectra, Far infrared radiation, Reprints, *Hydroxyl radials, Laser magnetic resonance.

The frequencies, wavelengths, and line strengths for transitions of the (18)OH molecule at microwave and far-infrared frequencies have been calculated from an analysis of its far-infrared laser magnetic resonance spectrum.

*600,497*
**PB87-106068** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Sensitive Comparison of Inner-Vacancy and Stripped Ion Spectra with Theory.**
Final rept.,
R. D. Deslattes, and E. G. Kessler. 1984, 11p
Pub. in Proceedings of International Conference on X-Ray and Inner-Shell Processes in Atoms, Molecules and Solids, Leipzig, East Germany, August 20-25, 1984, p165-175.

Keywords: *Electron transitions, X rays, Electronic spectra, One electron ions.

There are converging lines of theoretical and experimental progress in regard to rigorous comparisons between theory and experiment both for one-electron ions up to the region near Z=30 and for single vacancy x-ray transitions throughout the periodic table. Among the more important contributions to this progress are improved connections to the optical region (i.e., the Rydberg constant), enhanced ability to produce one-electron spectra over a significant range of Z, and the availability of all Z relativistic self consistent field calculations which are both accurate and convenient to use. The available comparisons suggest that (1) experiment and theory are consistent for low Z one-electron atoms, (2) experiment and theory are inconsistent for mid-to-high Z x-ray transitions, and (3) this inconsistency is probably not dominated by quantum electrodynamic contributions.

*600,498*
**PB87-106134** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Measurement of Liquid-Liquid Interfacial Kinetics.**
Final rept.,
G. J. Hanna, and R. D. Noble. 1985, 16p
Pub. in Chemical Reviews 85, n6 p583-598 1985.

Keywords: *Interfacial tension, Mass transfer, Reprints, *Liquid phases, *Chemical reaction kinetics.

Literature covering measurement of liquid-liquid interfacial kinetics, interfacial concentration measurement, and modeling of interfacial kinetics is reviewed. 85 References.

*600,499*
**PB87-107074** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Computer Matching Two Different Images of the Same Particle Field.**
Final rept.,
D. S. Bright. 1984, 2p
Pub. in Proceedings of the Annual Conference on Microbeam Analysis Society (19th)--Microbeam Analysis 1984, Bethlehem, PA, July 16-20, 1984, p173-174.

Keywords: Particles, *Microbeam analysis, Computer applications.

No abstract available.

*600,500*
**PB87-107132** PC **A02**
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Consecutive Ion Molecule Condensation-Reactions and Photodissociation Mechanisms of Condensation Ions in Polyacetylenic Compounds.**
Final rept.,
T. J. Buckley, L. W. Sieck, R. Metz, S. G. Lias, and J. F. Liebman. 1985, 16p
Pub. in International Jnl. of Mass Spectrometry and Ion Processes 65, n1-2 p181-196 1985.

Keywords: Mass spectroscopy, Chemical reactions, Chemical radicals, Reprints, *Photodissociation, *Chemical reaction mechanisms, Ion-molecule collisions, Photoionization, Acetylene/cyano, Cyanogen, Acetylene/di, Ion cyclotron resonance spectroscopy.

Consecutive ion-molecule condensation and condensation/dissociation reactions in diacetylene, cyanoacetylene, and cyanogen have been examined in an ion cyclotron resonance spectrometer at pressures of about 0.000001 torr, and in a high pressure photoioization mass spectrometer at pressures of about 0.01 torr.

*600,501*
**PB87-107389** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Laser Diagnostics of Gas/Surface Interactions.**
Final rept.,
R. R. Cavanagh, D. S. King, and D. A. Mantell. 1984, 7p
Pub. in Proceedings of 1984 Annual Meeting of American Institute of Chemical Engineers, San Francisco, CA., November 25-30, 1984, 7p.

Keywords: *Surfaces, *Desorption, Gases, Interactions, Energy transfer, Platinum, Ruthenium, Nitrogen oxide(NO).

Laser probes of energy transfer at surfaces are providing a new picture of fundamental energy transfer processes. The application of such techniques to monitor the vibrational, rotational, translational, alignment, and spatial orientation which results from gas/surface interactions is discussed. Emphasis is placed on systems which reflect departure from equilibrium behavior.

*600,502*
**PB87-107777** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Simulation of Aerosol Agglomeration in the Free Molecular and Continuum Flow Regimes,**
G. W. Mulholland, R. D. Mountain, and H. Baum. Mar 86, 50p NBSIR-86/3342
Sponsored by Defense Nuclear Agency, Washington, DC.

Keywords: *Aerosols, *Agglomerates, Molecular structure, Reaction kinetics, Clustering, Brownian movement, Fractals, Fractal dimensions.

The formation of high temperature aerosol agglomerates is simulated by following the Langevin trajectory of each particle with the boundary condition that the particles stick upon collision. Both the free molecular and continuum flow are treated. A new derivation of the friction force of an agglomerate in the continuum

limit is developed based on the evaluation of the surface momentum flux at the Oseen flow limit. The agglomerates can be described as fractal, at least in regard to power law relationship between mass and size, with a dimensionality of 1.7-1.9 independent of the flow regime. The particle growth is shown to be much more rapid in the free molecular regime than in the continuum. The global kinetics are shown to be consistent with a similarity analysis of the coagulation equation with a modified coagulation coefficient. Comparison between the simulation and coagulation theory at small time suggests a slight fluctuation enhancement in the free molecule case and a small-time enhancement of the coagulation rate at high concentration for the continuum case.

*600,503*
**PB87-108122** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Least Endothermic Fragmentation Pathways of the Diazine Cations.**
Final rept.,
R. Buff, and J. Dannacher. 1984, 15p
Pub. in International Jnl. of Mass Spectrometry and Ion Processes 62, n1 p1-15 1984.

Keywords: *Cations, *Diazine, Fragmentation, Endothermic reactions, Spectroscopy, Ions, Cleavage, Reprints, Energy conversion.

The least endothermic fragmentation pathways of the diazine cations have been investigated by variable residence time photoelectron-photoion coincidence spectroscopy. A detailed RRKM analysis of the corresponding results provides the rate energy functions for the loss of N sub 2 from the 1,2-diazine-and for the loss of HCN from the 1,3- and 1,4-diazine cations. The outcome of the analysis further implies that the processes in question involve a rate determining cleavage of the aromatic rings with a critical energy of approx. 2.7 eV and a correspondingly loose transition state. Quantitative accord between computed and measured rates can only be achieved when it is assumed that the reactions occur on the ground state manifold of the respective parent ions, suggesting rapid internal conversion of any initial excess electronic energy.

*600,504*
**PB87-108403** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Predicting Transport Properties without Adjustable Parameters: A Test Application of the Hulburt-Hirschfelder Potential to Argon.**
Final rept.,
P. M. Holland, L. Biolsi, and J. C. Rainwater. 1985, 6p
Pub. in Chemical Physics 99, p383-388 1985.

Keywords: *Transport properties, *Argon, Diffusion, Thermal conductivity, Viscosity, Gases, Reprints, Hulburt-Hirschfelder potential.

Accurate estimates of the transport properties of gaseous systems under conditions where experimental transport data are sparse or unavailable are important in a number of applications. The Hulburt-Hirschfelder (HH) potential for monatomic gas interactions, which is determined entirely by spectroscopic constants of diatomic molecules, provides a basis for calculating transport properties without adjustable parameters. In the paper the authors report test calculations of the viscosity, thermal conductivity and self-diffusion coefficients for argon. Comparison with the comprehensive correlation of thermophysical properties for argon by Kestin and co-workers shows very reasonable agreement for the transport properties at moderate and high temperatures. Deviations at lower temperatures may be attributed to inaccuracies in the long-range part of the HH potential, whereas the core and well of the potential appear to be adequately represented. These results strongly support the use of the HH potential for estimating the transport properties of monatomic gases at high temperatures.

*600,505*
**PB87-108411** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Thermal Conductivity of Ethane at Temperatures between 110 and 325 K and Pressures to 70 MPa.**
Final rept.,
H. M. Roder, and C. A. N. de Castro. 1985, 8p
Pub. in High Temperatures-High Pressures 17, p453-460 1985.

Keywords: *Ethane, *Thermal conductivity, Temperature, Density, Reprints.

New experimental measurements of the thermal conductivity of ethane for seventeen temperatures between 110 and 325 K at pressures to 70 MPa and densities to 22 mol dm sup-3 are presented. The measurements were made with a transient hot wire apparatus and cover a wide range of physical states including the dilute gas, the moderately dense gas, the near critical region, the compressed liquid states, and the vapor at temperatures below the critical temperature. A curve fit of the thermal conductivity surface allows comparison of the present results with others and with other correlations. The precision (two standard deviations) of the measurements is between 0.5% and 0.8% for wire temperature transients of 4-5 K, while the accuracy is estimated to be + or - 1.6%.

*600,506*
**PB87-108437** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Effect of External Mass-Transfer Resistance on Facilitated Transport.**
Final rept.,
R. D. Noble, J. D. Way, and L. A. Powers. 1986, 3p
Contract DE-AC21-84MC21271
Sponsored by Department of Energy, Washington, DC.
Pub. in Industrial and Engineering Chemistry Fundamentals 25, n3 p450-452 1986.

Keywords: *Mass transfer, Mathematical models, Membranes, Resistance, Reprints, *Liquid membranes, *Facilated transport, Carrier mediated transport.

An analytical expression is derived for the facilitation factor in facilated transport across a liquid film. The expression accounts for external mass-transfer resistances as well as diffusion and reaction within the liquid film. Evaluation of Sherwood numbers encountered in hollow-fiber membrane systems indicates the importance of external mass-transfer resistance. A graphical method based on the equation is presented and compared to experimental results.

*600,507*
**PB87-108445** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Kinetic Efficiency Factors for Facilitated Transport Membranes.**
Final rept.,
R. D. Noble. 1985, 9p
Pub. in Separation Science and Technology 20, n7-8 p577-585 1985.

Keywords: *Membranes, *Kinetics, Mathematical models, Reprints, *Faciliated transport, Efficiency factors, Carrier mediated transport.

A kinetic efficiency factor (eta) is defined for facilitated transport membranes. Eta is defined as the actual facilitated flux divided by the facilitated flux under reaction equilibrium conditions. Eta is correlated with an inverse Damkohler number epsilon. A dimensionless equilibrium constant K and mobility ratio alpha also affect the value of eta. Eta is shown to be useful in determining the operating regime of the system, comparing actual performance to maximum attainable, and providing a qualitative measure of the time to reach steady-state conditions.

*600,508*
**PB87-108452** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Mathematical Modeling of Facilitated Liquid Membrane Transport Systems Containing Ionically Charged Species.**
Final rept.,
J. P. Leiber, R. D. Noble, J. D. Way, and B. R. Bateman. 1985, 26p
Pub. in Separation Science and Technology 20, n4 p231-256 1985.

Keywords: *Mathematical models, Diffusion, Chemical reactions, Numerical analysis, Membranes, Reprints, *Liquid membranes, Facilitated transport, Carrier mediated transport.

A numerical model is presented which solves the transient nonlinear system of partial differential equations governing the facilitated transport of ionically charged species through a liquid membrane. The mathematical model is derived in dimensionless form and solved numerically. Facilitation factors and electrical potentials across the membrane are computed and compared to experimental results. This model is useful in predicting transient concentration, flux, and electrical potential gradients provided that the values of the required physical constants are known. It was noticed that transient facilitation factors are not affected by the transient electrical potential buildup, which indicated that both the pure diffusion and the facilitated transport of permeate are affected equally by the electrical effects of the ionically charged species.

*600,509*
**PB87-108601** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Far Infrared Laser Magnetic Resonance Detection of NH and ND (a (sup 1 Delta)).**
Final rept.,
K. R. Leopold, K. M. Evenson, and J. M. Brown. 1 Jul 86, 7p
Pub. in Jnl. of Chemical Physics 85, n1 p324-330, 1 Jul 86.

Keywords: *Spectroscopic analysis, Rotational spectra, Excitation, Hyperfine structure, Reprints, *Electronic structure, Laser magnetic resonance.

Rotational spectra of the excited a (sup 1 Delta) state of NH and ND have been observed by far infrared laser magnetic resonance spectroscopy. For ND A (sup1 Delta) the spectroscopic constants are B sub 0 = 264.750.263(30)MHz,Do = 13.383 83(91) MHz, (a sub N) = 109.63(22) MHz, (a sub D) = 11.03(23) MHz, eqQ(N) = -4.0(15) MHz,gr = -0.000 86(10), and gl = 1.000 506(17). For NH a (sup1 Delta), the constants are (B sub 0) = 493 043.182(95) MHz,D sub 0 = 50.453 MHz (constrained in fit), (a sub N) = 109.65(85) MHz,(a sub H) = 70.9(14) MHz,eqQ(N) = -4.0 MHz(constrained in fit), (g sub r) = -0.001 58(6), and (g sub L) = 1.001 03 (constrained in fit). Aspects of the electronic structure of the radical as revealed by the magnetic hyperfine constants are discussed in relation to those of chemically similar systems. The Zeeman parameters are interpreted in terms of mixing of the a (sup1 Delta) state with the c sup II state.

*600,510*
**PB87-108643** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Calculation of Phase Equilibria in Nitrogen-Ethane Mixtures by Extended Corresponding States.**
Final rept.,
K. D. Romig, and H. J. M. Hanley. Jan 86, 6p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Cryogenics 26, p33-38 Jan 86.

Keywords: *Phase transformations, *Ethane, *Nitrogen, Thermodynamics, Cryogenics, Phase diagrams, Reprints, Binary mixtures.

The phase diagram for the nitrogen-ethane mixture is determined via the extended corresponding states one-fluid theory. The authors support the contention that the mixture is a Type III mixture with a three-phase (liquid-liquid-vapour) line. The line can be calculated extremely well if binary interaction factors are fitted to the three-phase data. Without further adjustment, the liquid-liquid equilibrium (LLE) and vapour-liquid equilibrium (VLE) for the system are predicted satisfactorily. The parameters used, however, are not sufficient to predict satisfactory VLE data near a mixture critical line. The conclusion is in agreement with our previous work.

*600,511*
**PB87-109500** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**First and Second Dissociation Constants of Deuterio-o-Phthalic Acid in D20 from 5 to 50 C.**
Final rept.,
Y. C. Wu, and W. F. Koch. 1986, 13p
Pub. in Jnl. of Solution Chemistry 15, n6 p481-493 1986.

Keywords: Thermodynamic properties, Heavy water, Concentration(Composition), Isotope effect, Reaction kinetics, Reprints, *Dissociation constants, *Phthalic acid/deuterio, Activity coefficient, Thermodynamic activity.

The first and second dissociation constants of deuterio-o-phthalic acid in deuterium oxide have been determined by the emf method over the temperature range of 5 to 50 deg C. The pD values for potassium deuterium phthalate have been calculated from these two constants and experimentally verified. The thermodynamic properties for the dissociation of deuterio-o-phthalic acid have been evaluated.

*600,512*
**PB87-109518** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Thermodynamic Properties of DCl in D20 Solution from 5 to 50 C.**
Final rept.,
Y. C. Wu, W. F. Koch, and G. Marinenko. 1986, 20p
Pub. in Jnl. of Solution Chemistry 15, n8 p675-692 1986.

Keywords: *Hydrogen chloride, *Heavy water, Thermodynamic properties, Enthalpy, Entropy, Free energy, Electrochemical cells, Specific heat, Isotope effect, Reprints, *Deuterium chloride, Heat capacity.

The themodynamic properties of solutions of deuterium chloride (DCl) in deuterium oxide (D2O) have been determined from emf measurements of the electrochemical cell without transference from 5 to 50 deg C, and from 0.002 to 1.0/mol-kg. The standard potential of the silver/silver chloride electrode relative to the platinum/deuterium electrode has been determined. An equation for the Gibbs energy as a function of temperature has been derived from which the enthalpy, entropy, and heat capacity have been computed. Equations for the activity coefficient and the osmotic coefficient of DCl in D2O have been developed. The excess Gibbs energy of the solution and the excess partial molar free energy as a function of temperature have been calculated, from which the other excess thermodynamic properties have been computed. The solvent isotope effect on the excess thermodynamic functions is discussed.

*600,513*
**PB87-109641** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Spectrum and Energy Levels of the Sodiumlike Ion Sr(27+).**
Final rept.,
J. Reader. Jun 86, 4p
Pub. in Jnl. of the Optical Society of America B 3, n6 p870-873 Jun 86.

Keywords: *Molecular spectra, *Atomic enery levels, Plasma radiation, X rays, Reprints, *Strontium ions, *Ionization energy, Sodiumlike ions, Laser-produced plasma.

The spectrum of Sr(27+) was observed with a laser-produced plasma and a 2.2-m grazing-incidence spectrograph in the region 12-160 A. From the identification of 37 lines a system of 27 energy levels of the type 2p6nl was determined. The level system includes the configurations ns(n=3-5), np(n=3-6), nd(n=3-7), nf(n=4-6), and 5g. The ionization energy is determined as 11 188 200 + or - 1000/cm (1387.16 + or - 0.12 eV).

*600,514*
**PB87-109658** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Stark Broadening Along Homologous Sequences of Singly Ionized Noble Gases.**
Final rept.,
T. L. Pittman, and N. Konjevic. 1986, 7p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 35, n4 p247-253 1986.

Keywords: *Rare gases, *Stark effect, Neon, Argon, Krypton, Xenon, Plasma radiation, Reprints, Line broadening, Plasma spectroscopy.

The authors report measured Stark widths for eight Ne II, eight Ar II, five Kr II, and seven Xe II spectral lines, all belonging to np-nd doublets. A low-pressure, pulsed arc was used as a plasma source. Electron densities determined with an He-Ne laser quadrature interferometer cover the range 0.9 - 1.4 x 10 to the 23rd power/cu m. Electron temperatures, in the range 23,000 - 28,500 K, were measured by using the relative intensities of O II impurity lines. Experimental data for Ne II and Ar II agree well with the results of semiclassical calculations, where the average ratio of measured to calculated data is 0.96. The authors show that the analyzed results of the experimental data for np-nd doublets, within multiplets and supermultiplets along homologous sequences, are in close agreement with those presented in an earlier study.

*600,515*
**PB87-109674** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Thermal Conductivity of Methane-Ethane Mixtures at Temperatures between 140 and 330 K and at Pressures up to 70 MPa.**
Final rept.,
H. M. Roder, and D. G. Friend. Nov 85, 11p
Pub. in International Jnl. of Thermophysics 6, n6 p607-617 Nov 85.

Keywords: *Methane, *Ethane, *Thermal conductivity, Thermophysical properties, Reprints, Binary mixtures, Augmentation, Hot wires.

The paper presents new measurements on the thermal conductivity of three methane-ethane mixtures with methane mole fractions of 0.69, 0.50, and 0.35. The thermal conductivity surface for each mixture is defined by up to 13 isotherms at temperatures between 140 and 330 K with pressures up to 70 MPa and densities up to 25 mol/L. The measurements were made with a transient hot-wire apparatus. They cover a wide range of physical states including the dilute gas, the single-phase fluid at temperatures above the maxcondentherm, the compressed liquid states, and the vapor at temperatures below the maxcondentherm. The results show an enhancement in the thermal conductivity in the single-phase fluid down to the maxcondentherm temperature, as well as in the vapor and in the compressed liquid. A curve fit of the thermal conductivity surface is developed separately for each mixture.

*600,516*
**PB87-109690** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Vapor-Liquid Equilibrium of Near-Critical Binary Alkane Mixtures.**
Final rept.,
J. C. Rainwater, and F. R. Williamson. Jan 86, 10p
Pub. in International Jnl. of Thermophysics 7, n1 p65-74 Jan 86.

Keywords: Critical point, Thermophysical properties, Hexane, Pentane, Propane, Butane, Reprints, *Vapor liquid equilibrium, *Binary mixtures.

The modified Leung-Griffiths model of Rainwater and Moldover is used to correlate vapor-liquid equilibrium (VLE) surfaces in pressure, temperature, and density for binary mixtures in the near-critical region. The systems studied are butane-pentane, propane-isopentane, butane-hexane, and ethane-butane. The model, which has also successfully fit several other mixtures, is based on scaling-law equations of state expressed in terms of field variables. It incorporates a variation of the principle of corresponding states as well as the coupling of density and composition change across the phase boundary. As the width of the dew-bubble curves increases, additional parameters are required to obtain successful VLE correlations.

*600,517*
**PB87-109732** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Autoionization in a Fluctuating Electric Field.**
Final rept.,
K. Rzazewski, and J. Cooper. Jun 86, 4p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of the Optical Society of America B 3, n6 p891-894 Jun 86.

Keywords: *Electric fields, Variations, Ionization, Reprints, *Autoionization, *Plasma, Fluctuating microfield.

A simple model of autoionization in a fluctuating electric field is proposed and solved for the ionization rate. The fluctuating electric field can be a microfield in a plasma. Both dilute and dense plasmas are considered. Explicit expressions for broadening the Fano profile are derived and discussed in both cases, and particularly simple results are obtained in the impact limit.

*600,518*
**PB87-109906** Not available NTIS
American Chemical Society, Washington, DC.
**Journal of Physical and Chemical Reference Data, Volume 15, Number 2, 1986.**
Quarterly rept.
c1986, 437p
See also PB87-109914 through PB87-109955, and PB86-204567. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: *Research, Thermodynamic properties, Entropy, Enthalpy, Molecular vibration, Chemical reactions, Aromatic hydrocarbons, Aromatic monocyclic hydrocarbons, Equations of state, Density, Ethylene, Vapor pressure, Nitrogen, Solubility, *Foreign technology, Chemical reaction kinetics, Heat capacity, Polychlorinated biphenyls.

Table of contents include: Thermodynamic properties of twenty-one monocyclic hydrocarbons; Evaluated kinetic data for high-temperature reactions. Volume 5. Part 1. Homogeneous gas phase reactions of the hydroxyl radical with alkanes; Thermodynamic properties of ethylene from the freezing line to 2000 K at Pressures to 1000 MPa; A critical review of aqueous solubilities, vapor pressures, Henry's law constants, and octanol-water partition coefficients of the polychlorinated biphenyls.

*600,519*
**PB87-109914** Not available NTIS
American Chemical Society, Washington, DC.
**Thermodynamic Properties of Twenty-One Monocyclic Hydrocarbons,**
O. V. Dorofeeva, L. V. Gurvich, and V. S. Jorish.
c1986, 28p
Prepared in cooperation with Akademiya Nauk SSSR, Moscow. Inst. Vysokikh Temperatur. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n2 p437-464 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: *Aromatic monocyclic hydrocarbons, *Thermodynamic properties, Molecular structure, Molecular vibration, Entropy, Enthalpy, Free energy.

The available structural parameters, fundamental frequencies, and relative energies of different stable conformers, if any, for cyclopropane, cyclopropene, cyclobutane, cyclobutene, 1,3-cyclobutadiene, cyclopentane, cyclopentene, 1,3-cyclopentadiene, cyclohexane, cyclohexene, 1,3-cyclohexadiene, 1,4-cyclohexadiene, cycloheptane, cycloheptene, 1,3-cycloheptadiene, and 1,3,5,7-cyclooctatetraene were critically evaluated and the recommended values selected. Molecular constants for some molecules were estimated as the experimental values for these compounds are not available. This information was utilized to calculate the ideal gas thermodynamic properties C sub p,S,-(G-H sub 0)/T, H - H sub 0, and log K sub f from 100 to 1500K.

*600,520*
**PB87-109922** Not available NTIS
Leeds Univ. (England). Dept. of Physical Chemistry.
**Evaluated Kinetic Data for High-Temperature Reactions. Volume 5. Part 1. Homogeneous Gas Phase Reactions of the Hydroxyl Radical with Alkanes,**
D. L. Baulch, M. Bowers, D. G. Malcolm, and R. T. Tuckerman. c1986, 128p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n2 p465-592 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: Thermodynamics, Chemical radicals, Chemical reactions, Aliphatic hydrocarbons, Aromatic hydrocarbons, Methane, Ethane, Butane, Hexane, Heptane, *Chemical reaction kinetics, *Hydroxyl radicals, Butane/dimethyl, Pentane/methyl.

The available kinetic data for the homogeneous gas phase reactions of the hydroxyl radical with alkanes have been compiled and critically evaluated. For each reaction, relevant thermodynamic data, a table of

measured rate constants, a discussion of the data, and a comprehensive bibliography are presented. Wherever possible the preferred rate parameters are given with their associated error limits and temperature ranges.

*600,521*
**PB87-109930** Not available NTIS
Idaho Univ., Moscow. Center for Applied Thermodynamic Studies.
**Thermodynamic Properties of Ethylene from the Freezing Line to 450 K at Pressures to 260 MPa,**
M. Jahangiri, R. T. Jacobsen, and R. B. Stewart.
c1986, 141p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n2 p593-734 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: *Ethylene, *Thermodynamic properties, Enthalpy, Vapor pressure, Specific heat, Entropy, Density, Equations of state.

A new fundametnal equation explicit in Helmholtz energy for thermodynamic properties of ethylene from the freezing line to 450 K at pressures to 260 MPa is presented. Independnt equations for the vapor pressure for the saturated liquid and vapor densities as functions of temperature, and for the ideal gas heat capacity are also included. The fundamental equation was selected from a comprehensive function of 100 terms on the basis of a statistical analysis of the quality of the fit. The fundamental equation and the derivative functions for calculating internal energy, enthalpy, entropy, isochoric heat capacity (Cv), isobaric heat capacity (Cp), and velocity of sound are included. The fundamental equation reported here may generally be used to calculate pressures and densities with an uncertainty of + or - 0.1%, heat capacities within + or - 3%, and velocity of sound values within + or - 1%. Comparisons of calculated properties to experimental data are included to verify the accuracy of the formulation.

*600,522*
**PB87-109948** Not available NTIS
Idaho Univ., Moscow. Center for Applied Thermodynamic Studies.
**Thermodynamic Properties of Nitrogen from the Freezing Line to 2000 K at Pressures to 1000 MPa,**
R. T. Jacobsen, R. B. Stewart, and M. Jahangiri.
c1986, 171
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n2 p735-909 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: *Thermodynamic properties, *Nitrogen, Density, Enthalpy, Entropy, Equations of state, Specific heat, Tables(Data), Heat capacity, Temperature dependence, Pressure dependence.

A new fundamental equation explicit in Helmholtz energy for thermodynamic properties of nitrogen from the freezing line to 2000 K at pressures to 1000 MPa is presented. New independent equations for the vapor pressure and for the saturated liquid and vapor densities as functions of temperature are also included. Tables of thermodynamic properties of nitrogen are given for liquid and vapor states within the range of validity of the fundamental equation.

*600,523*
**PB87-109963** Not available NTIS
American Chemical Society, Washington, DC.
**Journal of Physical and Chemical Reference Data, Volume 15, Number 3, 1986.**
Quarterly rept.
c1986, 349p
See also PB87-109971 through PB87-110029, and PB86-204567. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research, Thermochemical properties, Titanium chlorides, Thermodynamic properties, Iron, Silicon, Enthalpy, Entropy, Standards, Thermal conductivity, Toluene, Heptane, Methane, Combustion, Ion-molecule collisions, Computer applications, Electron photon interactions, Photoionization, Photodissociation, Ion clusters, Standard reference materials, Chemical reaction kinetics.

Table of contents includes the following: Computer methods applied to the assessment of thermochemical data. Part 1. The establishment of a computerized thermochemical data base illustrated by data for TiCl4(g), TiCl4(l), TiCl3(cr), and TiCl2(cr); Thermodynamic properties of Iron and Silicon; Cross Sections for collisions of electrons and photons with nitrogen molecules; Thermochemical data on gas-phase ion-molecule association and clustering reactions; Standard reference data for the thermal conductivity of liquids; Chemical kinetic data base for combustion chemistry. Part 1. Methane and related compounds; Cumulative listing or reprints and supplements.

*600,524*
**PB87-109971** Not available NTIS
Sussex Univ., Brighton (England). School of Chemistry and Molecular Sciences.
**Computer Methods Applied to the Assessment of Thermochemical Data. Part 1. The Establishment of a Computerized Thermochemical Data Base Illustrated by Data for TiCl4(g), TiCl4(l), TiCl3(cr), and TiCl2(cr),**
S. P. Kirby, E. M. Marshall, and J. B. Pedley. c1986, 23p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n3 p943-965 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Titanium chlorides, *Thermochemical properties, Enthalpy, Heat of formation, Entropy, Computer applications.

Computer methods are described for the storage, retrieval, and processing of large amounts of thermochemical data and related textual material. The procedures are illustrated by a critical evaluation of data for TiCl4(g), TiCl4(1), TiCl3(cr), and TiCl2(cr); values for standard enthalpies of formation and entropies at 298.15 K are selected for these species.

*600,525*
**PB87-109989** Not available NTIS
Center for Information and Numerical Data Analysis and Synthesis, Lafayette, IN.
**Thermodynamic Properties of Iron and Silicon,**
P. D. Desai. c1986, 17p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n3 p967-983 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermodynamic properties, *Iron, *Silicon, Enthalpy, Specific heat, Vapor pressure, Gibbs free energy, Heat capacity.

The work reviews and discusses the data on the various thermodynamic properties of iron and silicon available through March 1984. These include heat capacity, enthalpy, enthalpies of transition and melting, vapor pressure, and enthalpy of vaporization. The recommended values for heat capacity, enthalpy, entropy, and Gibbs energy function cover the temperature range from 1 to 3200 K for iron and 1 to 3600 K for silicon. The recommended values for vapor pressure cover the temperature range from 298.15 to 3200 K for iron and from 298.15 to 3600 K for silicon. These values are referred to temperatures based on the International Practical Temperature Scale o

*600,526*
**PB87-109997** Not available NTIS
Institute of Space and Astronautical Science, Tokyo (Japan).
**Cross Sections for Collisions of Electrons and Photons with Nitrogen Molecules,**
Y. Itikawa, M. Hayashi, A. Ichimura, K. Onda, and K. Sakimoto. c1986, 27p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n3 p985-1010 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Nitrogen, Cross sections, Excitation, Elastic scattering, Molecular vibration, *Electron-molecule collisions, *Photon-molecule collisions, Photoionization, Photodissociation, Electron collisions.

Data have been compiled on the cross sections for collisions of electrons and photons with nitrogen molecules(N2). For electron collisions, the processes considered are: total scattering, elastic scattering, momentum transfer, excitations of rotational, vibrational and electronic states, dissociation, and ionization. Ionization and dissociation processes are discussed for photon impact. Cross section data selected are presented graphically. Spectroscopic and other properties of the nitrogen molecule are summarized. The literature was surveyed through the end of 1984, but some more recent data are included when useful.

*600,527*
**PB87-110003** Not available NTIS
Pennsylvania State Univ., University Park. Dept. of Chemistry.
**Thermochemical Data on Gas-Phase Ion-Molecule Association and Clustering Reactions,**
R. G. Keesee, and A. W. Castleman. c1986, 61p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n3 p1011-1071 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermodynamic properties, Enthalpy, Entropy, Free energy, Chemical reactions, Dissociation energy, *Ion-molecule collisions, *Ion clusters.

A comprehensive tabulation of the standard enthalpy change, delta H, entropy change, delta S, and free energy change delta G, for the formation of ion clusters from ion-molecule association reactions is given. The experimental methods which are used to derive the data are briefly discussed. For some experiments, dissociation energies of ion clusters are reported and listed under the category of delta H. The relationship between delta H and dissociation energy is discussed in the text.

*600,528*
**PB87-110011** Not available NTIS
Lisbon Univ. (Portugal). Dept. de Quimica.
**Standard Reference Data for the Thermal Conductivity of Liquids,**
C. A. Nieto de Castro, S. F. Y. Li, N. Nagashima, R. D. Trengove, and W. A. Wakeham. c1986, 14p
Prepared in cooperation with Imperial Coll. of Science and Technology, London (England). Dept. of Chemical Engineering and Chemical Technology, and Keio Univ., Yokohama (Japan). Dept. of Mechanical Engineering. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n3 p1073-1086 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermal conductivity, *Water, *Toluene, *Heptane, Thermodynamic properties Liquids, Convection, Concentric cylinders.

The available experimental liquid-phase thermal conductivity data for water, toluene, and n-heptane have been examined with the intention of establishing standard reference values along the saturation line. The quality of available data is such that for toluene and water new standard reference values can be proposed with confidence limits better than + or - 1.0% for most of the normal liquid range. For n-heptane there are insufficient reliable experimental data for the system to be treated as a primary reference standard, so a lower quality correlation has been developed which yields a set of secondary reference data with confidence limits of + or - 1.5% for most of the normal liquid range.

*600,529*
**PB87-110110** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Photoelectron-Photoion Coincidence Study of the Bromobenzene Ion.**
Final rept.,
H. M. Rosenstock, R. Stockbauer, and A. C. Parr. 15 Jul 80, 5p
Pub. in Jnl. of Chemical Physics 73, n2 p773-777, 15 Jul 80.

Keywords: Photoelectrons, Mass spectroscopy, Fragmentation, Reprints, *Electron-ion collisions, *Benzene/bromo, *Photoionization, Phenyl radicals.

The technique of variable time photoelectron-photoion coincidence mass spectrometry has been applied to the fragmentation of bromobenzene ion producing a phenyl ion. A detailed analysis of the variation of the breakdown curve with parent ion residence time was performed. The results lead to phenylion = 270 kcal/mole in close agreement with recalculated results from an earlier study on chlorobenzene. This, combined with other photoionization results leads to phenyl radical = 83 plus or minus 3 kcal/mole, slightly higher than the value 80.9 plus or minus 2 kcal/mole obtained from neutral kinetics. The analysis leads to a rate-energy dependence for the fragmentation process and an equivalent 1000 K Arrhenius pre-exponential factor of 9.4 x 10 to the 14th power/sec, which may be compared to the value 2 x 10 to the 14th power/sec for the analogous neutral process. The possible contribution of spin orbit splitting is discussed.

*600,530*

**PB87-110185** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Resonant Electron and Ion Emission and Desorption Mechanism in Rare Earth Oxides.**
Final rept.,
J. Schmidt-May, F. Senf, J. Voss, C. Kunz, and A. Flodstroem. 1985, 12p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Surface Science 163, p303-314 1985.

Keywords: *Desorption, Chemisorption, Rare earth compounds, Reaction kinetics, Surface chemistry, Reprints, *Samarium oxides, *Europium oxides, *Ytterbium oxides, Ion emission, Photoelectron spectroscopy.

The resonant enhancement in photoelectron spectra at the 4d edges of rare earth atoms and metals is also found in yield spectra of desorbed ions from the surfaces of the oxides of Sm, Eu and Yb following the photon excitation. The analysis of the 4 -> 4f resonance leads to a picture of an indirect mechanism of ion desorption which is mainly caused by the flux of energetic 4f photoelectrons from the bulk. In this case the dominant desorption through secondary processes limits the use of the photon-stimulated desorption (PSD) to determine to which type of atom the desorbing species was attached.

*600,531*

**PB87-110193** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Recent Developments in Quantitative Surface Analysis by Electron Spectroscopy.**
Final rept.,
C. J. Powell. 1986, 8p
Pub. in Jnl. of the Vacuum Science and Technology A4, n3 p1532-1539 May/Jun 86.

Keywords: *Electron spectroscopy, *Chemical analysis, Surface chemistry, Calibration, Reprints.

An overview is given of recent developments in quantitative surface analysis by x-ray photoelectron spectroscopy and Auger electron spectroscopy. The two major tasks of an analysis are the identification of the surface phases that are present and the determination of the concentrations of particular elements or compounds. Methods for accomplishing both tasks are described together with the pitfalls and problems that remain. Particular attention is given to the following topics: identification of surface phases and reference data for the calibration of instrumental energy scales; reference data on inelastic mean free paths and attenuation lengths; effects of specimen crystallinity; intensity measurements; measurement of the imaging properties of electron energy analyzers; and the intensity-energy response functions of different instruments.

*600,532*

**PB87-111050** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Photofragmentation Dynamics of Acetone at 193 nm: State Distributions of the CH3 and CO Fragments by Time- and Wavelength-Resolved Infrared Emission.**
Final rept.,
D. J. Donaldson, and S. R. Leone. 1986, 8p
Contract DOE-EA-77-A-01-6010, Grant NSF-PHY82-00805
Sponsored by Department of Energy, Washington, DC., and National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 85, n2 p817-824, 15 Jul 86.

Keywords: *Acetone, *Photolysis, Chemical radicals, Excitation, Carbon monoxide, Infrared radiation, Vibration, Rotation, Reprints, *Methyl radicals.

The photolysis of acetone at 193 nm is known to produce two methyl radicals and CO following excitation of a (sup1 (n,3s)) Rydberg transition. Vibrational excitation is detected in both products immediately following the dissociating laser pulse by observing the resulting infrared emission. Vibrational distributions are obtained for CH (nu sub 3) and for CO. These are, for CH (nu sub 3) nu=1/2/3=0.73 + or - 0.05/0.13 + or - 0.05/0.13 + or 0.05 and for CO nu =1/2/3=0.75 + or - 0.05/0.16 + or -0.05/0.09 + or -0.05. An approximate rotational temperature of 1500 K can be used to fit the CH3(nu sub 3) emission spectrum. The CO is formed with very high, non-Boltzmann rotational excitation. The result strongly suggests that the three-body dissociation occurs via a two-step mechanism, rather than a rigorously concerted process. The high rotational excitation is most likely imparted by the kinematics in the breakup of a bent acetyl fragment.

*600,533*

**PB87-111076** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Electron-Impact Ionization of Mg-Like Ions: S(4+), C1(5+), and Ar(6+).**
Final rept.,
A. M. Howald, D. C. Gregory, F. W. Meyer, R. A. Phaneuf, and N. Djuric. 1986, 8p
Contract DE-AC05-84OR21400
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Physical Review A 33, n6 p3779-3786 Jun 86.

Keywords: Excitation, Cross sections, Reprints, *Magnesiumlike ions, *Electron-ion collisions, Autoionization, Sulfur ions, Chlorine ions, Argon ions, Crossed beams, *Ionization cross sections.

Absolute electron-impact ionization cross sections were measured as a function of collision energy for ions in the Mg-isoelectronic sequence S(4+), C(5+), and Ar(6+). The measurements cover the energy range from threshold to 1500 eV and show onsets due to the indirect ionization process of innershell excitation followed by autoionization. The relative magnitude of the indirect ionization process increases dramatically in comparison with the direct process along the sequence, a feature which is also emphasized by earlier data for Al(1+).

*600,534*

**PB87-113619** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Viscosity of Light and Heavy Water and Their Mixtures.**
Final rept.,
J. Kestin, N. Imaishi, S. H. Nott, J. C. Nieuwoudt, and J. V. Sengers. 1985, 21p
Contract DE-AC02-81ER10811
Sponsored by Department of Energy, Washington, DC.
Pub. in Physica 134A, p38-58 1985.

Keywords: *Heavy water, *Water, *Viscosity, Measurement, Mixtures, Reprints.

The paper presents measurements of the viscosity of light and heavy water and their mixtures at temperatures between 25C and 220C and at pressures from the saturation pressure up to 30MPa. A comparison with the international formulations for the viscosity of fluid H2O and D2O adopted by the International Association for the Properties of Steam reveals some systematic differences from the previously accepted values for the viscosity of liquid D2O. A unified representative equation is proposed which yields the viscosity of mixtures of liquid H2O and D2O at all concentrations, at temperatures from the freezing point up to 350C, and at pressures up to approximately 100 MPa.

*600,535*

**PB87-113627** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Boundary Layer Effects in Facilitated Transport Liquid Membranes.**
Final rept.,
R. D. Noble, J. D. Way, and L. A. Powers. 1986, 4p
Pub. in American Institute of Chemical Engineers Symposium Series 82, n248 p94-97 1986.

Keywords: Mass transfer, Mathematical models, Separation, Reprints, *Liquid membranes, *Faciliated transport.

An analytical expression is derived for the facilitation factor in facilitated transport across a liquid film. The expression accounts for external mass-transfer resistances as well as diffusion and reaction within the liquid film. Comparison with experimental results is very good.

*600,536*

**PB87-114930** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Ion Broadening of Ar I Lines in a Plasma.**
Final rept.,
D. W. Jones, W. L. Wiese, and L. A. Woltz. 1986, 7p
Pub. in Physical Review A 34, n1 p450-456 Jul 86.

Keywords: *Argon, Line spectra, Line width, Stark effect, Reprints, *Line broadening.

The authors have measured the profiles of plasma-broadened, slightly red-shifted spectral lines of neutral argon with a wall-stabilized arc and performed a detailed line-shape analysis with a computerized data acquisition and processing system. In full agreement with the quasistatic theory of ion broadening, the authors' experiment shows asymmetry patterns with characteristic minima and maxima near the central part of the lines. While the positions of these extrema--as well as the zero crossing point--stay essentially constant for all lines when compared on a reduced wavelength scale, the amplitudes of the extrema vary from line to line. Measurements of the amplitudes thus allow, by comparison with theoretical asymmetry patterns, the determination of ion broadening parameters.

*600,537*

**PB87-115218** PC **A07**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Bibliographies of Industrial Interest: Thermodynamic Measurements on the Systems CO2-H2O, CuCl2-H2O, H2SO4-H2O, NH3-H2O, H2S-H2O, ZnCl2-H2O, and H3PO4-H2O.**
Final rept.,
B. R. Staples, D. Garvin, D. Smith-Magowan, T. L. Jobe, and J. Crenca. Sep 86, 149p NBS/SP-718
Also available from Supt. of Docs as SN003-003-027-68-5. Library of Congress catalog card no. 86-600544.
Sponsored by American Inst. of Chemical Engineers, New York.

Keywords: *Thermodynamic properties, *Bibliographies, Specific heat, Enthalpy, Ammonia, Carbon dioxide, Copper chlorides, Hydrogen sulfide, Phosphoric acid, Sulfuric acid, Zinc chlorides, Equilibrium, *Binary mixtures.

Contained herein are bibliographies of sources of experimental and correlated thermodynamic data for seven binary aqueous mixtures of industrial importance, namely mixtures of CO2, H2S, NH3, H2SO4, H3PO4, CuCl2 and ZnCl2 with water. The categories of equilibrium data included in the bibliographies are activity and osmotic coefficients, equilibria in solution, enthalpies and heat capacity data, vapor-liquid equilibria, and phase equilibrium data.

*600,538*

**PB87-116232** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Automation of the NBS (National Bureau of Standards) Threshold Photoelectron-Photoion Coincidence Mass Spectrometer.**
Final rept.
J. J. Butler, D. M. P. Holland, A. C. Parr, R. Stockbauer, and R. Buff. 1985, 4p
Pub. in Jnl. of Physics E: Scientific Instruments 18, p286-289 1985.

Keywords: *Mass spectrometers, Chemical analysis, Automation, Reprints, Threshold photoelectrons, Time-of-flight spectrometers, Photoions.

The pulse counting and delay circuitry for a threshold photoelectron-photoion coincidence mass spectrometer is presented along with the automation system using a DEC LSI 11/23 computer and CAMAC instrumentation. A switching output register and logic circuits are used to measure alternately a time of flight coincidence mass spectrum and a background accidental spectrum, at selected photon energies. The high voltage, fast rise time pulse used for time of flight analysis creates special signal isolation problems which are handled with unique pulse blanking techniques.

*600,539*
**PB87-116240** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Photoelectron Branching Ratios and Asymmetry Parameters of the Two Outermost Molecular Orbitals of Methyl Cyanide.**
Final rept.,
D. M. P. Holland, A. C. Parr, and J. L. Dehmer. 1984, 10p
Grant NATO-1939
Sponsored by Office of Naval Research, Arlington, VA., Department of Energy, Washington, DC., and North Atlantic Treaty Organization, Brussels (Belgium).
Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 34, p87-96 1984.

Keywords: *Atomic orbitals, Atomic energy levels, Photoelectrons, Reprints, *Cyanide/methyl, Photoionization.

Vibrationally resolved photoelectron branching ratios and asymmetry parameters have been determined for the two outermost molecular orbitals of methyl cyanide. The results are discussed briefly within the context of similar studies on cyanogen and hydrogen cyanide, and in relation to structures exhibited in the photoionization efficiency curve.

*600,540*
**PB87-117693** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Multiphoton Ionization Spectroscopy of ClO and BrO.**
Final rept.,
M. T. Duignan, and J. W. Hudgens. 1985, 8p
Pub. in Jnl. of Chemical Physics 82, n10 p4426-4433 1985.

Keywords: Excitation, Mass spectra, Reprints, *Multiphoton ionization, *Bromine monoxide, *Chlorine monoxide, Electronic structure, Ryberg states.

The authors report the resonance enhanced multiphoton ionization spectra of ClO and BrO between 415 and 475 nm. The observed electronic states were prepared by simultaneous absorption of three identical photons from a dye laser. Absorption of at least one additional photon induced ionization. ClO showed spectra originating from the D, E, and F states. BrO showed three new vibrational progressions originating from transitions between the X (sup2)Pi(sub3/2) state to Rydberg states with assignments of E (sup2)sigma ( nu(sub 00) = 65003/cm), F (sup2)sigma (nu(sub 00) = 67470/cm), and an apparently inverted multiplet state designated G (nu(sub 00 = 70504/cm). The G-state bands were separated by 139 (+ or - 3) cm which should approximate the magnitude of the spin-orbit coupling constant of the excited state if it is of (sup2)Pi(subi) symmetry.

*600,541*
**PB87-118105** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Thermodynamics of Ammonium Scheelites II. Heat Capacity of Deuterated Ammonium Perrhenate ND4Re04 from 7.5 to 320 K.**
Final rept.,
R. J. C. Brown, J. E. Callanan, R. D. Weir, and E. F. Westrum. 1986, 6p
Sponsored by Michigan Univ., Ann Arbor. Dept. of Chemistry, and Royal Military Coll. of Canada, Kingston (Ontario).
Pub. in Jnl. of Chemical Thermodynamics 18, p787-792 1986.

Keywords: *Specific heat, Scheelite, Thermodynamic properties, Metaliferous minerals, Reprints, *Heat capacity, *Deuterated ammonium perrhenate.

The heat capacity of the scheelite salt deuterated ammonium perrhenate ND4ReO4 was measured from 7.5 to 320 K without detection of any phase transition. An anomalous peak found between 270 and 280 K resulted from fusion of a saturated solution of D2O trapped in the lattice. Values of the standard molar thermodynamic quantities for pure ND4ReO4 are presented up to 320 K.

*600,542*
**PB87-118139** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Dependence of Pressure in a Bubbler Tube on Liquid Properties.**
Final rept.,
A. K. Gaigalas. 1982, 8p
Pub. in American Institute of Chemical Engineers Jnl. 28, p922-929 1982.

Keywords: *Liquids, Density, Cross sections, Calibration, Reprints, *Pressure dependence, Bubbler tubes.

An experiment was performed to study the dependence of pressure (P) in a bubbler tube on liquid properties. For a given mass of liquid in a tank of uniform cross-sectional area A, the pressure in the bubbler tube depends on liquid temperature, density, surface tension, bubble size, and heel volume, which is the space between the bottom of the tank and the tip of the bubbler tube. The relationship for the pressure was found to be consistent with all measurements. In a second part of the investigation a cylindrical tank was calibrated with water at room temperature. The calibration was extrapolated to measure the volume of water at 40 deg C and uranyl nitrate ar 20 deg C and 40 deg C. All measurements indicated that the extrapolation procedure discussed in the study is valid. The sensitivity of the extrapolation to density changes and tank geometry changes is presented.

*600,543*
**PB87-118303** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Hydrogen Component Fugacities in Binary Mixtures with Carbon Dioxide.**
Final rept.,
T. J. Bruno, and G. L. Hume. 1986, 11p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in International Jnl. of Thermophysics 7, n5 p1053-1063 1986.

Keywords: *Hydrogen, *Carbon dioxide, Thermophysical properties, Reprints, Fugacity coefficients, Binary mixtures, Gas mixtures.

The fugacity coefficients of hydrogen in binary mixtures with carbon dioxide were measured using a physical equilibrium technique. The technique involves the use of an experimental chamber which is divided into two regions by a semipermeable membrane. Hydrogen can penetrate and pass through the membrane, while the other component (in this case carbon dioxide) cannot. At equilibrium, pure hydrogen will permeate into one 'compartment' of the chamber, while the binary mixture occupies the other compartment. Thus, the pressure of pure hydrogen on one side of the membrane approaches the partial pressure of hydrogen in the mixture on the other side of the membrane. This allows the direct measurement of the hydrogen component fugacity at a given mixture mole fraction. In this study, results are reported for measurements made on the hydrogen+carbon dioxide binary at 80 deg C (355 K), 130 deg C (403 K), 160 deg C (433 K), and 190 deg C (463 K).

*600,544*
**PB87-118311** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Hydrogen Component Fugacities in Binary Mixtures with Methane and Propane.**
Final rept.,
T. J. Bruno, G. L. Hume, and J. F. Ely. 1986, 19p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in International Jnl. of Thermophysics 7, n5 p1033-1051 1986.

Keywords: *Hydrogen, *Methane, *Propane, Thermophysical properties, Reprints, Fugacity coefficients, Binary mixtures, Gas mixtures.

The fugacity coefficients of hydrogen in binary mixtures with methane and propane were measured using a physical equilibrium technique. The technique involves the use of an experimental chamber which is divided into two regions by a semipermeable membrane. Hydrogen can penetrate and pass through the membrane, while the other component (in this case, methane or propane) cannot. At equilibrium, pure hydrogen will permeate into one 'compartment' of the chamber, while the binary mixture occupies the other compartment. Thus, the pressure of pure hydrogen on one side approaches the partial pressure of hydrogen in the mixture on the other side of the membrane. In the study, results are reported for measurements made on the hydrogen+propane binary at 80 deg C (353 K) and 130 deg C (403 K) and the hydrogen+methane binary at 80 deg C (353 K). All measurements were performed with a total mixture pressure of 3.45 MPa.

*600,545*
**PB87-118337** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Multiphone Excitation of Autoionizing States of Mg: Line-Shape Studies of the 3p2 singlet S State.**
Final rept.,
R. E. Bonanno, C. W. Clark, and T. B. Lucatorto. 1986, 4p
Contract DE-AI01-85ER60302
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A 34, n3 p2082-2085 Sep 86.

Keywords: Excitation, Reprints, *Magnesium atoms, *Autoionization, Multi-photon processes, Resonance ionization mass spectrometry.

The authors have observed ionization of Mg by both direct and stepwise two-photon excitation of the 3p(2) Singlet S state. The line shape of the single-color direct process is strongly modified by the resonance denominator associated with the intermediate virtual state. The measured energy and width of this resonance as determined by the stepwise two-color technique agree well with previous determinations.

*600,546*
**PB87-118626** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Migration of Population to Higher-Angular-Momentum Rydberg States through the Degenerate Raman Coupling.**
Final rept.,
R. Grobe, G. Leuchs, and K. Rzazewski. 1986, 7p
Pub. in Physical Review A: General Physics 34, n2 p1188-1194 Aug 86.

Keywords: Atomic energy levels, Reprints, *Rydberg states, Hydrogen atoms.

A model is formulated which describes migration of population from low-l to higher-l states of the same principal quantum number in the highly excited state of the atom. The physical mechanism is the degenerate, nearly resonant Raman coupling. Specific calculations are performed for the hydrogen atom. The laser light is modeled as a monochromatic coherent or chaotic colored noise.

*600,547*
**PB87-118683** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Thermodynamic Properties of Isobutane-Isopentane Mixtures.**
Final rept.,
J. S. Gallagher, and J. M. H. Levelt Sengers. 1984, 6p
Sponsored by Department of Energy, San Francisco, CA. San Francisco Operations Office.
Pub. in Transactions - Geothermal Resources Council 8, p59-64 1984.

Keywords: *Thermodynamic properties, Equations of state, Enthalpy, Reprints, *Pentane/iso, *Butane/iso, Binary mixtures.

A Helmholtz function for mixtures of isobutane and isopentane has been formed based upon a recent correlation of pure isobutane as the reference fluid and using extended corresponding states principles. The function can be used to generate other thermodynamic properties of interest by differentiations with respect to its independent variables V,T, and X. Sample tables

of properties generated in the way and a pressure-enthalpy chart of interest to the designer of geothermal power cycles are presented.

*600,548*
**PB87-118717** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**PVT Properties of Methanol at Temperatures to 300 deg C.**
Final rept.,
G. C. Straty, A. M. F. Palavra, and T. J. Bruno. 1986, 13p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in International Jnl. of Thermophysics 7, n5 p1077-1089 1986.

Keywords: *Methyl alcohol, Carbinols, Compressibility, Density, Pressure, Volume, Temperature, Reprints, *Compressed gas.

Measurements of the PVT behavior of compressed gas and liquid methanol are reported. Pressure versus temperature observations were made along paths of very nearly constant density (pseudoisochores) in the temperature range from about 100 to 300 deg C and at pressures to about 35 MPa. Eighteen pseudoisochores were determined, ranging in density from about 2 to 22 mol/cu dm.

*600,549*
**PB87-118725** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Test of the Mean Density Approximation for Lennard-Jones Mixtures with Large Size Ratios.**
Final rept.,
J. F. Ely. 1986, 13p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in International Jnl. of Thermophysics 7, n2 p381-393 Mar 86.

Keywords: Computerized simulation, Reprints, *Lennard-Jones mixtures, Molecular dynamics.

The mean density approximation for mixture radial distribution functions plays a central role in modern corresponding-states theories. This approximation is reasonably accurate for systems that do not differ widely in size and energy ratios and which are nearly equimolar. As the size ratio increases, however, or if one approaches an infinite dilution of one of the components, the approximation becomes progressively worse, especially for the small molecule pair. In an attempt to better understand and improve this approximation, isothermal molecular dynamics simulations have been performed on a series of Lennard Jones mixtures. Thermodynamic properties, including the mixture radial distribution functions, have been obtained at seven compositions ranging from 5 to 95 mol %. The results of the simulations are compared with the mean density approximation and a modification to integrals evaluated with the mean density approximation is proposed.

*600,550*
**PB87-119582** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Heterodyne Frequency Measurements on the Nitric Oxide Fundamental Band.**
Final rept.,
A. Hinz, J. S. Wells, and A. G. Maki. 1986, 6p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Molecular Spectroscopy 119, p120-125 1986.

Keywords: *Nitric oxide(NO), *Molecular spectra, Band spectra, Frequency measurement, Reprints.

Heterodyne frequency measurements have been made on the fundamental band of nitric oxide from 1750 to 1931/cm. Based on the analysis of these new measurements, minor changes are made in the band constants and an improved list of calculated energy levels for the nu = 0 and nu = 1 states is given.

*600,551*
**PB87-119764** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Thermodynamic Property Formulation for Ethylene from the Freezing Line to 450 K at Pressures to 260 MPa.**
Final rept.,
M. Jahangiri, R. T. Jacobsen, R. B. Stewart, and R. D. McCarty. 1986, 11p
Pub. in International Jnl. of Thermophysics 7, n3 p491-501 1986.

Keywords: *Thermodynamic properties, *Ethylene, Equations of state, Reprints.

A new thermodynamic property formulation based upon a fundamental equation explicit in Helmholtz energy of the form A=A(rho, T) for ethylene from the freezing line to 450 K at pressures to 260 MPa is presented. A vapor pressure equation, equations for the saturated liquid and vapor densities as functions of temperature, and an equation for the ideal-gas heat capacity are also included. The fundamental equation and the derivative function for calculating internal energy, enthalpy, entropy, isochoric heat capacity (C sub v), isobaric heat capacity (C sub P), and velocity of sound are included. The fundamental equation reported here may be used to calculate pressures and densities with an uncertainty of plus or minus 0.1%, heat capacities within plus or minus 3%, and velocity of sound values within plus or minus 1%, except in the region near the critical point.

*600,552*
**PB87-119772** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Orthobaric Liquid Densities and Dielectric Constants of Carbon Dioxide.**
Final rept.,
W. M. Haynes. 1986, 6p
Pub. in Advances in Cryogenic Engineering 31, p1199-1204 1986.

Keywords: *Carbon dioxide, *Density(Mass/volume), Dielectric properties, Reprints, *Dielectric constant.

Measurements of the orthobaric liquid densities and dielectric constants of carbon dioxide have been obtained at temperatures between 220 and 300 K. Densities were determined with a magnetic suspension densimeter, while a concentric cylinder capacitor was used for measurements of dielectric constant. The experimental densities and dielectric constants have been used to compute values for the Clausius-Mossotti function. Comparisons with the experimental results of other investigators are presented.

*600,553*
**PB87-119780** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Dissociation of Diatomic Molecules at Metal Surfaces.**
Final rept.,
J. W. Gadzuk, and S. Holloway. 1985, 4p
Pub. in Chemical Physics Letters 114, n3 p314-317 1985.

Keywords: *Dissociation, Surface chemistry, Reprints, *Metal surfaces, *Diatomic molecules.

No abstract available.

*600,554*
**PB87-119798** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Vibrational Lineshapes of Adsorbed Molecules.**
Final rept.,
J. W. Gadzuk, and A. C. Luntz. 1984, 22p
Pub. in Surface Science 144, n2-3 p429-450 1984.

Keywords: *Surface chemistry, Vibrational spectra, Adsorption, Molecules, Reprints.

The possible information content in lineshapes observed in vibrational spectroscopy of molecules adsorbed on surfaces is considered by drawing analogies with similar situations in other spectroscopic areas where the systematics are more completely understood. Particular emphasis is placed on the relative roles of T(sub 1) (dissipative decay) vs. T'(sub 2) (pure dephasing) processes in determining linewidths, on the roles of substrate electron-hole pairs, phonons, and photons in T(sub 1) processes, and possible ways to establish which broadening mechanism is operative in a given situation. A particular kind of dephasing that is important for vibrational lineshapes in molecular crystals, so called exchange-coupling, is suggested as playing a significant role for molecular adsorbates as well. Some recent experimental studies are analyzed in the light of concepts introduced in the paper.

*600,555*
**PB87-119806** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Energy Redistribution and Dissociation in Molecule-Surface Collisions Involving Charge Transfer/Surface Hopping.**
Final rept.,
S. Holloway, and J. W. Gadzuk. 1985, 13p
Pub. in Surface Science 152-153,n2 p838-850 1985.

Keywords: *Surface chemistry, Surfaces, Excitation, Dissociation, Vibration, Adsorption, Reprints, *Molecule collisions, Charge transfer.

In analogy with resonance electron scattering from molecules in which substantial high vibrational overtone losses are observed, beams of diatomic molecules scattered from solid surfaces could emerge highly vibrationally excited due to the formation of temporary negative molecular ions resulting from charge transfer between the solid and molecule on the inward and outward legs of the scattering trajectory. In the present work, the exact classical trajectories for the diatomic molecule, including internal vibrational motion, are calculated for motion over model diabatic potential surfaces in which surface hopping due to charge transfer/harpooning is accounted for. From these calculations, the probability for translational to vibrational energy transfer are obtained as a function of incident kinetic energy and system parameters.

*600,556*
**PB87-120010** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Van der Waals Potentials from the Infrared Spectra of Rare Gas-HF Complexes.**
Final rept.,
G. T. Fraser, and A. S. Pine. 1986, 14p
Pub. in Jnl. of Chemical Physics 85, n5 p2502-2515, 1 Sep 86.

Keywords: *Hydrogen fluoride, *Rare gases, Infrared spectra, Reprints, *Binding energy, Van der Waals forces, Tunable lasers.

High-resolution infrared spectra of the Ar-HF, Kr-HF, and Xe-HF van der Waals molecules have been recorded in the vicinity of the H-F stretching fundamentals nu sub 1 under thermal equilibrium conditions at T approx. 211 K with a tunable difference-frequency laser. Rotational structure has been observed up to or approaching rotational predissociation, permitting us to model the effective radial van der Waals potentials for these complexes. These potentials provide good estimates for the binding energies, D(sub 0) and the van der Waals stretching frequencies nu sub 3, in the ground (nu sub 1 = 0) and excited (nu sub 1 = 1) states of the molecules.

*600,557*
**PB87-120028** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Vibrational Population Lifetimes of OH(v=1) in Natural Crystalline Micas.**
Final rept.,
E. J. Heilweil. 1986, 7p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Chemical Physics Letters 129, n1 p48-54, 15 Aug 86.

Keywords: *Mica, Infrared spectra, Muscovite, Nonmetalliferous minerals, Hydrogen bonds, Crystal structure, Biotite, Reprints, *Vibrational lifetime, Picosecond pulses.

Picosecond infrared saturation-recovery measurements have been performed on the OH-stretching vibrations (3500-3710/cm) of hydroxyl groups located within the octahedral layers of ten naturally occurring crystalline micas. At room temperature, the average OH(nu = 1) vibrational population lifetime (T1 plus or minus sigma for OH(1-) in muscovite is 92 plus or minus 13 ps. For biotite samples, absorptions arising from two distinct lattice sites yield T1=221 plus or minus 23 and 87 plus or minus 33 ps, respectively. Crystal structures, hydroxyl orientation and hydrogen

bonding, ionic environment and infrared spectroscopy of these mineral families are used to rationalize the observed relaxation times.

*600,558*
**PB87-120226** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Photodissociation of Vinyl Chloride: Formation and Kinetics of Vinylidene H2CC((3)B2).**
Final rept.,
A. Fahr, and A. H. Laufer. 1985, 4p
Pub. in Jnl. of Physical Chemistry 89, n13 p2906-2909 1985.

Keywords: *Vinyl chloride, Chlorine organic compounds, Excitation, Concentration(Composition), Photolysis, Reprints, *Photodissociation, *Chemical reaction kinetics, *Vinylidene, Rate constants.

The primary photodissociation processes in the photolysis of vinyl chloride have been investigated using the flash photolysis-kinetic spectroscopic technique. Concentrations and temporal profiles of product H2CC((3)B2), HC1 and C2H2 are monitored by their absorption in the vacuum ultraviolet at 137, 139 and 151 nm, respectively. HC1 and H2CC((3)B2) are formed with the same time history via a 1,1 elimination from excited C2H3C1. Rate constants for the interaction of H2CC((3)B2) with He, 1.07 plus or minus 0.17 x 10 to the -14th power cc/molec s, and C2H3C1, 3.5 x 10 to the 11th power cc/molec s, have been obtained.

*600,559*
**PB87-121331**
(Order as PB87-121315, PC **A04**/MF **A01**)
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Triple Point of Oxygen in Sealed Transportable Cells,**
G. T. Furukawa. 19 Mar 86, 21p
Included in Jnl. of Research of the National Bureau of Standards, v91 n5 p255-275 Sep-Oct 86.

Keywords: *Oxygen, Calorimeters, Calibration, Phase transformations, Thermodynamic properties, *Triple points.

The triple points of oxygen samp'es sealed in miniature pressure cells were investigated by means of adiabatic calorimetry. The triple point of a 99.999 percent pure commercial oxygen sample was found to be 0.94 mK higher than that of an 'ultra-pure' sample prepared by thermal decomposition of potassium by thermal decomposition of potassium permanganate (KMnO4). The capsule-type platinum resistance thermometers that have been used are shown to have outstanding stability and the multiple calibrations made on them at the National Bureau of Standards extending over six years are shown to be consistent to within 0.15 mK at 54.361K. The results of measurements on an internationally circulated sealed cell of commercial oxygen show its temperature to by 0.58(sub 1) mK higher than those of the ultra-pure oxygen.

*600,560*
**PB87-122248** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Differential Techniques of Kinetic Analysis of DSC (Differential Scanning Calorimetry) Data for Thermal and Photopolymerization Reactions.**
Final rept.,
J. H. Flynn. 1984, 5p
Pub. in Proceedings of North American Thermal Analysis Society Conference (13th), Philadelphia, PA., September 23-26, 1984, p229-233.

Keywords: *Reaction kinetics, Curing, Chemical reactions, Thermal analysis, Polymerization, *Photopolymerization, Differential scanning calorimetry.

The kinetics of bulk thermal or photochemical cure of resins are typically complex. Interpretation of the initial phase is beclouded by induction periods and irregular activation of radical initiators. Differential scanning calorimetry is ideal for monitoring these reactions as the amplitude is a robust measure of the rate of change in the enthalpy of propagation step--often the opening of a double bond to form a polymer linkage. Because of the above mentioned complexities it is prudent to perform isothermal measurement of these processes. Therefore, the paper develops isothermal differential techniques in which the rate is described as a function of time. Also, a quick method for estimating 'reaction order' from ratios of times to reach various fractions of an arbitrary initial rate is described. The above methods are illustrated by examples from photo and thermal cure DSC experiments.

*600,561*
**PB87-122339** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electron Devices Div.
**Advanced Integrated Test Structure for High Speed Measurement of Generation Lifetime.**
Final rept.,
D. McCarthy, M. G. Buehler, J. Acevedo, B. Stamps, and M. Lonky. 1978, 3p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Extended Abstracts, Electrochemical Society Fall Meeting, 1978, Monterey, CA., November 14-16, 1978, p488-490.

Keywords: *Electrochemistry, Semiconductor diodes, Lifetime(Durability), Silicon.

An integrated test circuit, consisting of a reverse biased gated diode connected to a source-follower MOSFET amplifier, was developed to rapidly measure the generation lifetime in a p-n junction. As many as 540 junctions were measured on a 55 mm diameter silicon wafer where the measurement time was less than 0.5 s per structure. Circuit models were developed which indicate how to design the circuit so as to simplify the analysis.

*600,562*
**PB87-122354** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Calculation of Thermal Degradation Initiated by Random Scission. 1. Steady-State Radical Concentration.**
Final rept.,
A. Inaba, and T. Kashiwagi. 1986, 8p
Pub. in Macromolecules 19, n9 p2412-2419 Sep 86.

Keywords: *Thermal degradation, Concentration(Concentration), Molecular weight, Mathematical models, Chemical radicals, Reprints.

Changes in molecular weight distribution and in sample volume were calculated for thermal degradation of a polymer. The thermal degradation scheme consists of random scission initiation, depropagation, and disproportionation termination reactions. A steady-state radical concentration was used in the study. The initial molecular weight distribution of the sample was expressed by a logarithmic normal distribution. Results were obtained in two ways: one was by approximate analytical solutions describing changes in molecular weight and in the sample volume, including effects of initial polydispersity of the sample; the other was by numerical calculation. Comparison among the analytical solutions obtained in the study, previously published solutions, and the numerically calculated results indicates that the solutions obtained in the study can apply to more general initial molecular weight distributions and agree better with the numerical results than previously published results. Effects of initial molecular weight, average zip length, initial polydispersity, and order of the termination reaction on changes in molecular weight, polydispersity, and the volume of the sample are discussed.

*600,563*
**PB87-122370** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Polarization Switching Versus Optical Bistability: Experimental Observations for a J(sub lower) = 1 to J(sub upper) = 0 Transition in a Fabry-Perot Cavity.**
Final rept.,
C. Parigger, P. Hannaford, and W. J. Sandle. 1986, 16p
Pub. in Physical Review A 34, n3 p2058-2072 Sep 86.

Keywords: Optical pumping, Reprints, *Samarium atoms, Optical bistability, Polarization.

Experiments on the steady-state, nonlinear behavior of the (sup 7)F(1)-(sup 7)F(0) 570.68-nm transition of atomic samarium in a laser-driven, near-concentric Fabry-Perot cavity are reported. For zero applied magnetic field, only simple optical bistability, symmetric in both sigma(+) and sigma(-) transmitted polarization, is observed for a linearly polarized excitation beam. However, for a magnetic field applied parallel to the propagation direction, polarization-sensitive switching appears, with lowest power threshold near the edge of the Doppler-broadened region. Subsidiary measurements of atomic parameters are also given to enable the transition to be experimentally well characterized.

*600,564*
**PB87-122388** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Electron Affinities of the Alkali Halides and the Structure of Their Negative Ions.**
Final rept.,
T. M. Miller, D. G. Leopold, K. K. Murray, and W. C. Lineberger. 1986, 8p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 85, n5. p2368-2375, 1 Sep 86.

Keywords: *Haloalkanes, Molecular structure, Ground states, Reprints, *Electron affinity, Photoelectron spectroscopy, Negative ions.

Photoelectron spectra are reported for the MX(X tilde (sup 1 Sigma)(1+))+e(1-)<-MX-(1-) X tilde (sup 2 Sigma(1+)) transitions of ten alkali halide anions at 488 nm. Adiabatic electron affinities (plus or minus 0.010 eV) are determined to be 0.593 (LiC1), 0.520 (NaF), 0.727 (NaC1), 0.788 (NaBr), 0.865 (NaI), 0.582 (KCl), 0.642 (KBr), 0.728 (KI), 0.543 (RbCl) and 0.455 eV (CsCl). Fundamental vibrational frequencies, equilibrium bond lengths, and dissociation energies are also reported for the anion sup 2 Sigma(1+) ground states. An observed linear correlation of electron affinities with alpha/r(sup 2) (alpha = metal atom polarizability) is used to predict the electron affinities of the remaining alkali bromides and iodides, as well as related alkali salts. A simple electrostatic model for the alkali halide anions is also presented which enables the accurate (plus or minus 0.1 eV) calculation of electron affinities.

*600,565*
**PB87-122396** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Reaction Mechanism and Kinetics of Silane Pyrolysis on a Hydrogenated Amorphous Silicon Surface.**
Final rept.,
R. Robertson, and A. Gallagher. 1986, 8p
Sponsored by Solar Energy Research Inst., Golden, CO.
Pub. in Jnl. of Chemical Physics 85, n6 p3623-3630, 15 Sep 86.

Keywords: *Silicon, Silane, Pyrolysis, Surface chemistry, Substrates, Reprints, *Chemical reaction kinetics, Amorphous silicon.

Three regimes of pressure and temperature are identified in which silane pyrolysis has distinctly different initial kinetics: in two regimes the initial reactions are heterogeneous and in the third regime it is homogeneous. The authors report here a preliminary model for the heterogeneous reaction regime where the decomposition rate is nearly independent of pressure. In the model the silicon surface is saturated with hydrogen and hence is nonreactive. The rate limiting step for silane decomposition is the creation of reactive surface sites by release of hydrogen. These reactive sites are refilled by decomposition of SiH4 or reincorporation of H2. A new adsorbed state of SiH4 is proposed which is bound to the surface by a three-center bond. After making some simplifications to the full model the kinetics are solved for static-and flowing-gas hot wall reactor experiments. The implications of the proposed reactions for the other two pyrolysis regimes and for silane discharges are briefly discussed.

*600,566*
**PB87-122412** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Impure Steam Near the Critical Point.**
Final rept.,
J. M. H. Sengers, C. M. Everhart, G. Morrison, and R. F. Chang. 1984, 11p
Pub in Proceedings of International Conference on the Properties of Steam (10th), Moscow, USSR, September 3-7, 1984 p277-287.

Keywords: *Steam, Thermodynamic properties, Sodium chloride, Specific heat, Critical point, Solutions, Impurities.

The thermodynamic properties of dilute near-critical mixtures are given according to a classical and a non-classical model. Measurements obtained in dilute solutions of NaCl in near-critical steam are discussed in the light of these models. Questions are raised regarding the validity near the critical point of extended Debye-Huckel formulations recently proposed by Pitzer et al.

*600,567*
**PB87-122420** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Photoinduced Evaporation of Charged Clusters.**
Final rept.,
P. C. Engelking. 1986, 8p
Pub. in Jnl. of Chemical Physics 85, n5 p3103-3110, 1 Sep 86.

Keywords: *Evaporation, *Carbon dioxide, Reprints, Clusters, Photodissociation.

The average cluster size remaining after photoinduced evaporation of a cluster of specific initial size can be predicted by an RRK/QET statistical model, provided that the correct average kinetic energy release is used. Theoretical justification for this correction, based upon detailed balance, is provided here. Agreement with experiments on (CO2(1+)sup n clusters at several wavelengths shows that for these aggregates the average bond strength above n=2 is approximately 3.6 plus or minus 0.6 kcal/mol.

*600,568*
**PB87-122446** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Approximate Rotational Band Shifts.**
Final rept.,
P. C. Engelking. 1986, 2p
Pub. in Jnl. of Physical Chemistry 90, n19 p4544-4545 1986.

Keywords: *Spectroscopic analysis, Band spectra, Rotational vibration, Reprints.

Interpretation of spectroscopic experiments in which the rotational lines are not resolved often requires an expression for the shift of the center of the rotational band. Previous expressions are corrected and extended to cases of linear, symmetric, spherical, and asymmetric rotors, with typical accuracy of a fraction of the rotational B constant.

*600,569*
**PB87-122479** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Band Broadening of CH2 Vibrations in the Raman Spectra of Polymethylene Chains.**
Final rept.,
S. L. Wunder, M. I. Bell, and G. Zerbi. 1986, 13p
Pub. in Jnl. of Chemical Physics 85, n7 p3827-3839, 1 Oct 86.

Keywords: Alkanes, Vibrational spectra, Raman spectra, Polymers, Reprints, *Line broadening, *Polymethylene.

The isotropic and anisotropic linewidths of methylene vibrations in a homologous series of alkanes of increasing chain length have been measured in the liquid state as a function of temperature. The bandwidths of the CH2 symmetric stretching modes, which are in Fermi resonance with overtones of the CH2 bending vibrations, are temperature insensitive over a 200 K interval; this is best explained in terms of a vibrational dephasing mechanism (inhomogeneous broadening) for these modes. In contrast, for the bending and antisymmetric stretching vibrations, significant band broadening occurs over this same temperature interval. In addition, for these modes, both the absolute value of the bandwidth and the relative rate of increase of the bandwidth with increasing temperature, decrease with increasing chain length. These observations are consistent with a reorientational broadening mechanism as the principal bandwidth contribution for these vibrations.

*600,570*
**PB87-122578** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Characterization of the Imaging Properties of a Double-Pass Cylindrical-Mirror Analyzer.**
Final rept.,
N. E. Erickson, and C. J. Powell. 986, 7p
Pub. in Surface and Interface Analysis 9, p111-117 1986.

Keywords: Surfaces, Electron beams, Electron energy, Reprints, *Photoelectron spectroscopy, Auger electron spectroscopy, Imaging techniques.

The imaging properties of a double-pass cylindrical-mirror analyzer have been investigated using extensions of the technique recently described by Seah and Mathieu. Elastic-peak intensity data obtained as an electron beam was rastered across a test specimen, was recorded in digital form and later used to generate 'three-dimensional' images. Images have been obtained for a range of operating conditions and for displacements of the specimen from its optimum position. Measured image widths were in semi-quantitative agreement with those expected from a simple analysis although deviations attributed to instrument imperfections were found. Elastic-peak images provide a convenient and quantitative means of assessing instrument performance and defining the specimen area being analyzed for the selected conditions.

*600,571*
**PB87-122586** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Dynamics of the Laser-Induced Thermal Desorption of Nitric Oxide from a Platinum Foil.**
Final rept.,
D. R. F. Burgess, D. A. Mantell, R. R. Cavanagh, and D. S. King. 1986, 2p
Contract DE-AI05-84ER13150
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Chemical Physics 85, n5 p3123-3124, 1 Sep 86.

Keywords: *Nitric oxide(NO), *Desorption, Platinum, Surface chemistry, Kinetic energy, Reprints, Time-of-flight method.

The internal and kinetic energy distributions of nitric oxide, which was desorbed from a cold polycrystalline platinum foil by laser-induced thermal desorption, were measured using a laser-excited fluorescence, time-of-flight technique. Under irradiation conditions which are estimated to produce a maximum surface temperature of 320 K, the desorbed NO was represented by two distributions of molecules: a translationally energetic component with a mean kinetic energy E(sub T) = 450 meV, a rotational temperature T(sub R) = 410 K, and a vibrational temperature T(sub V) = 800 K; and a slower component with E(sub T) = 57 meV and T(sub R) = 170 K.

*600,572*
**PB87-122594** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Surface Chemical Analysis - Report on the VAMAS (Versailles Project on Advanced Materials and Standards) Project.**
Final rept.,
C. J. Powell, and M. P. Seah. 1986, 5p
Contract DE-Alo5-84ER13150
Pub. in Jnl. of Chemical Physics 85, n5 p3123-3124, 1 Sep 86.

Keywords: *Surfaces, *Chemical analysis, Standards, Reprints, Reference materials, VAMAS project.

The VAMAS project on surface chemical analysis is a multi-national cooperation for the provision of standards data and materials for surface chemical analysis measurement and for the provision of the basic understanding necessary for these activities. The project is one of a rapidly growing suite of projects initiated as a result of decisions following the 1982 Versailles Summit Meeting of the Heads of State or Government of Canada, France, Germany, Italy, Japan, UK, USA and the representatives of the Commission of the European Communities. During the past year national representatives to the VAMAS project have been appointed and national committees established. The article summarizes the philosophy, scope, and organization of the project and describes specific activities that have been initiated. Information is given on how individuals, both within and outside the group of member states, may participate.

*600,573*
**PB87-122727** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Length and Mass Div.
**Electric Field Effects in Rydberg Atoms.**
Final rept.,
D. A. Harmin. 1985, 16p
Pub. in Comments on Atomic and Molecular Physics 15, n6 p281-296 1985.

Keywords: *Stark effect, Symmetry, Density, Atomic spectra, Reprints, Autoionization.

A comprehensive, nonperturbative theory of the dc Stark effect in non-hydrogenic atoms is outlined for any multichannel spectrum amenable to a quantum-defect analysis. The density of atomic states is obtained, through a geometrical transformation, in terms of atomic parameters and separate hydrogenic barrier effects.

*600,574*
**PB87-122735** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Length and Mass Div.
**Asymmetry of Field-Induced Shape Resonances in Hydrogen.**
Final rept.
D. A. Harmin. 1985, 7p
Pub. in Physical Review A 31, n5 p2984-2990 May 85.

Keywords: *Hydrogen, Resonance, Stark effect, Reprints.

Asymmetric resonance profiles observed in H atoms in a strong electric field are derived analytically. The most significant deviations from a Lorentzian lineshape, H sup F = gamma/e(sup Z) + gamma (sup Z), occur for resonances near the top of a potential barrier. Parametrization as a Fano profile is inappropriate. The lineshape formula, a Lorentzian with energy dependent reduced width gamma(sub Q) (e) = ln(1+Q(1-Q) (sup (-1-e))/ln(1-Q) (sub -1), depends on a single asymmetry parameter Q (0 plus or minus Q plus or minus 1).

*600,575*
**PB87-122768** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Theoretical Studies of Potential Gas-Phase Charge-Transfer Complexes: NH3 + HX (X = Cl, Br, I).**
Final rept.,
P. Jasien, and W. Stevens. 1986, 5p
Pub. in Chemical Physics Letters 130, n1-2 p127-131, 26 Sep 86.

Keywords: *Ammonia, Hydrogen bonds, Gases, Haloalkanes, Hydrogen bromide, Hydrogen chloride, Hydrogen iodide, Reprints, Charge transfer.

Theoretical calculations of the potential curves for the NH3 + HX systems (X = Cl, Br, I) predict only a single minimum for the HCl and HBr complexes, corresponding to the hydrogen-bonded structure. In the case of the HI complex, a double-well proton-transfer potential curve with a small barrier is found. The presence of the second minimum corresponding to the NH4(1+) I (1-) structure may result in an anomalous intensity and transition energy for excitation of the HI stretch in the NH3-HI complex.

*600,576*
**PB87-127999** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Use of Synchrotron Radiation to Measure Electron Attenuation Lengths in Condensed Molecular Solids.**
Final rept.,
R. Stockbauer, R. L. Kurtz, N. Usuki, and T. E. Madey. 1986, 5p
Pub. in Nuclear Instruments and Methods in Physics Research A246, p820-824 1986.

Keywords: *Surface chemistry, Photoelectrons, Thickness, Solids, Substrates, Reprints, Synchrotron radiation.

The authors describe a method for using synchrotron radiation to measure accurately electron attenuation lengths in condensed molecular solids as a function of electron energy. It consists of measuring the attenuation of photoelectrons from a well characterized, relatively inert, cooled surface as a condensable overlayer is deposited. As photoelectrons from the substrate

escape they pass through and are scattered in the overlayer. This scattering appears as a decrease in the intensity of the substrate photoelectron peak. The measurement of this decrease as a function of layer thickness gives the electron attenuation lengths directly. By using monochromatized synchrotron radiation for the photoemission excitation source, one can tune the photon energy and, hence, obtain the attenuation lengths as a function of electron kinetic energy. The techniques developed for obtaining a uniform overlayer film and for determining its thickness are given in detail. These techniques are applicable to most condensable samples that can be introduced into the vacuum system as a gas.

*600,577*
**PB87-128039** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**2s(2) 2p(5) - 2s 2p(6) Transitions in Fluorinelike Ions from Zr(31+) to SN(41+).**
Final rept.,
J. Reader, C. M. Brown, J. O. Ekberg, U. Feldman, and J. F. Seely. Nov 86, 3p
Contract DE-AI08-84-DP40092/26
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of the Optical Society of America B3, n11 p1609-1611 Nov 86.

Keywords: *Atomic energy levels, Excitation, Wavelengths, Zirconium, Tin, Plasma(Physics), Reprints, *Fluorinelike ions.

Transitions of the type 2s(2) 2p(5) - 2s2p(6) have been observed in eight fluorinelike ions from Z(31+) to Sn(41+). The spectra were produced by focusing light from the Nd:glass Omega laser at the University of Rochester onto solid targets and photographing the resultant plasmas with a 3-m grazing-incidence spectrograph. The identified transitions are in the region 24-60 A. The measured wavelengths are in good agreement with wavelengths calculated with the semiempirical formulas of Edlen (Phys.xScr. 28, 51 (1983). Wavelengths for the 2s(2) 2p(5) doublet P(sub 3/2) - doublet P(sub 1/2) magnetic-dipole transitions are given for each ion.

*600,578*
**PB87-128047** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Specific Heats (Cv) of Saturated and Compressed Liquid and Vapor Carbon Dioxide.**
Final rept.,
J. W. Magee, and J. F. Ely. 1986, 20p
Sponsored by National Research Council, Washington, DC.
Pub. in International Jnl. of Thermophysics 7, n6 p1163-1182 Nov 86.

Keywords: *Carbon dioxide, *Specific heat, Thermophysical properties, Reprints, *Heat capacity.

Specific heats of saturated liquid carbon dioxide (C sub sat) have been measured in the temperature range 220 to 303 K. Specific heats at constant volume (C sub v) have been measured at 12 densities ranging from 0.2 to 2.5 times the critical density in the temperature range 233 to 330 K, with pressures varying from 3.4 to 32 MPa. The measurements have been conducted in an adiabatic constant-volume calorimeter of conventional design. Uncertainty of the specific heats is estimated to not exceed 2.0%. Comparisons are made with an extended Benedict-Webb-Rubin equation of state and with the results of other workers.

*600,579*
**PB87-128096** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Gas-Phase Hydrolysis of SOF2 and SOF4.**
Final rept.,
R. J. Van Brunt, and I. Sauers. 1986, 4p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in Jnl. of Chemical Physics 85, n8 p4377-4380, 15 Oct 86.

Keywords: Hydrolysis, Reprints, *Chemical reaction kinetics, *Fluoride/thionyl, *Tetrafluoride/thionyl, Vapor phases.

The rates for gas-phase hydrolysis of SOF2 (thionyl-fluoride) and SOF4 (thionyl tetrafluoride) have been measured at a temperature of 298 K. The second order rate constant for SOF2 hydrolysis in SF6 buffer gas was found to have the value (1.2 + or - 0.3) x 10 to the -23 power cc/s which agrees with previous estimates of Sauers, et al., but is three orders of magnitude lower than the value obtained by Ruegsegger, et al. at 340 K. The rate constant for SOF4 hydrolysis has not previously been measured and its value in both SF6 and N2 buffer gases was found here to be (1.0 + or - 0.3) x 10 to the -21st power cc/s.

*600,580*
**PB87-128229** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Comparison of Some Thermodynamic Properties of H2O from 273.15 to 473.15 K as Formulated in the 1983 ASHRAE (American Society of Heating, Refrigerating and Air Conditioning Engineers) Tables and the 1983 NBS/NRC Steam Tables.**
Final rept.,
R. W. Hyland. 1985, 7p
Pub. in Proceedings of the International Symposium on Moisture Humidity, p29-35 1985.

Keywords: *Water, *Thermodynamic properties, Enthalpy, Entropy.

In 1983 two independent studies of the thermodynamic properties of saturated H2O were completed, one by Wexler and Hyland (WH) and a second by Haar, Gallagher, and Kell (HGK). WH includes only saturated phases for 173.15 < or = +0 T < or = +0 473.15 K, and is derived from fitting equations to data for particular parameters. HGK includes the entire thermodynamic surface over the temperature range 273.15 < or = +0 T < or = +0 2500 K and the pressure range O < or = +0 P < or = +0 3 x 10 to the 9th power Pa, and is derived from the Helmholz function. Because of the differences in approach and scope, it is of interest to compare the formulations in their region of overlap. The paper includes comparisons for the specific volumes, enthalpies, and entropies of the liquid and vapor states. Also given are comparisons for the vapor pressure and second virial coefficients. Generally, the agreement is within the stated uncertainties of the two formulations.

*600,581*
**PB87-128294** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Vibrational Predissociation of the Nitric Oxide Dimer: Total Energy Distribution in the Fragments.**
Final rept.,
M. P. Casassa, J. C. Stephenson, and D. S. King. 1986, 2p
Pub. in Jnl. of Chemical Physics 85, n4 p2333-2334, 15 Aug 86.

Keywords: *Nitrogen oxide(NO), *Dissociation, Vibration, Reprints, *Energy distribution, Van der waals forces.

Rotational-, spin-orbit-, lambda doublet-, and kinetic energy distributions were measured by laser-excited fluorescence techniques for the nitric oxide fragments formed from the vibrational predissociation of nitric oxide dimers in a free jet expansion. The NO fragments, produced following excitation in the dimer -nu sub 1 fundamental, were described by a rotational temperature of TR=102 K, with full equilibration of lambda doublet states, and a spin-orbit 'temperature' TSO=175 K. The velocity distributions were isotropic with an average fragment kinetic energy of 245/cm.

*600,582*
**PB87-128419** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Differential Techniques for the Kinetic Analysis of DSC Data.**
Final rept.,
J. H. Flynn. 1985, 4p
Pub. in Thermochimica Acta 92, p153-156 1985.

Keywords: Thermal analysis, Chemical reactions, Thermochemistry, Reprints, *Chemical reaction kinetics, Differential scanning calorimetry.

A simple technique for the kinetic analysis of rate vs. time data from an isothermal DSC experiment is presented. Selected ascending or descending sections of the rate curve are fitted to dq/dt = k(q sub 0 + or - q) (sub n). Values for n are determined and their consistency tested by the ratios of times to reach reduced rates of reaction.

*600,583*
**PB87-128427** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Temperature Gradients in Horizontal Tube Furnaces.**
Final rept.,
J. H. Flynn, and L. A. Dunlap. 1986, 4p
Pub. in Thermochimica Acta 105, p215-218 1986.

Keywords: *Temperature gradients, Thermal analysis, Temperature measurement, Calibrating, Temperature control, Laminar flow, Furnaces, Reprints.

Radial temperature differences in a 1 in. diameter horizontal tube furnace similar to those used in thermogravimetry were measured as a function of purge gas flow rate and pressure at temperatures from 25 to 525 deg C. The temperature difference between a thermocouple at the tube axis and one 0.8 cm off center was 45 deg C at 400 deg C, 1 atm pressure of nitrogen and 25 ml/min flow rate. The large temperature difference was attributed to laminar flow conditions. Effects of these large radial variations on temperature measurement and calibration are discussed. Several methods for minimizing these temperature differences by insertion of in-line preheaters and mixers are suggested.

*600,584*
**PB87-128443** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Thermoneutral Isotope Exchange Reactions in Proton-Bound Complexes of Water with Organic Molecules: Correlations with Energetics of Formation of the Corresponding Association Ions.**
Final rept.,
S. G. Lias. 1984, 7p
Pub. in Jnl. of Physical Chemistry 88, n19 p4401-4407 1984.

Keywords: Isotope exchange, Chemical reactions, Reprints, *Ion-molecule collisions, *Chemical reaction kinetics.

The efficiencies of the reaction: MH(1+) + D2O -> MD(1+) + HDO or the analogous reaction in which deuteration is reversed have been measured for the cases, M = formaldehyde, acetaldehyde, methanol, methyl formate, propionaldehyde, dimethylether, 1,4-dioxane, acetone, diethylether, di-n-propylether, and pyridine. A quantitative evaluation of the model used in estimating well depths leads to the conclusion that the energies of association in such complexes are primarily electrostatic in nature, since the model, which considers only electrostatic interactions, predicts well depths in close agreement with those obtained by experiment or ab initio calculations.

*600,585*
**PB87-128468** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Collisional Quenching of Excited Vinylidene ((3)B2) Radicals.**
Final rept.,
A. Fahr, and A. H. Laufer. 1986, 4p
Pub. in Jnl. of Physical Chemistry 90, n21 p5064-5067, 9 Oct 86.

Keywords: Excitation, Chemical radicals, Reprints, *Chemical reaction kinetics, *Vinylidene radicals, Rate constants, Quenching.

Rate constants for the removal of excited-state vinylidene D2CC ((3) B 2) in the presence of He, Ar, N2, H2, CO, and CH4 are reported at room temperature.

*600,586*
**PB87-128815** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Shear-Induced Phase Changes in Mixtures.**
Final rept.,
K. D. Romig, and H. J. M. Hanley. 1986, 9p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in International Jnl. of Thermophysics 7, n4 p877-885 Jul 86.

Keywords: *Phase transformations, *Shear tests, Mixtures, Thermophysical properties, Reprints.

A thermodynamic theory to account for the behavior of liquid mixtures exposed to a shear is developed. One consequence of the theory is that shear-induced phase changes are predicted. The theory is based on a thermodynamics that includes specifically the shear rate in the formalism and is applied to mixtures by a straightforward modification of the corresponding states, conformal-solution approach. The approach is general but is used here for a mixture of Lennard-Jones particles with a Lennard-Jones equation of state as a reference fluid. The results are discussed in the context of the Scott and Van Konynenberg phase classification. It is shown that the influence of a shear does affect substantially the type of the phase behavior. Results from the model mixture are equated loosely with those from real polymeric liquids.

*600,587*
**PB87-128823** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Extended Corresponding States as a Tool for the Prediction of the Thermodynamic Properties of Mixtures.**
Final rept.,
R. D. McCarty. 1986, 10p
Pub. in International Jnl. of Thermophysics 7, n4 p901-910 Jul 86.

Keywords: Themodynamic properties, Nitrogen, Methane, Ethane, Equations of state, Reprints, *Binary mixtures.

The principle of corresponding states, with one of its many extensions, is used to predict the thermodynamic properties of the binary mixtures N2-CH4 and CH4-C2H6. Comparisons of the predicted properties with experimental data are given to illustrate some of the powers and problems associated with the method. Problems encountered in modeling mixtures, which are not necessarily associated with the mathematical model of the equation of state, are also discussed. Wide-range equations of state for the two binary systems mentioned above are presented.

*600,588*
**PB87-128831** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Thermodynamic Behavior of Fluids Near the Critical Point.**
Final rept.,
J. V. Sengers, and J. M. H. Levelt Sengers. 1986, 34p
Pub. in Annual Review of Physical Chemistry 37, p189-222 1986.

Keywords: *Fluids, Thermophysical properties, Gravity, Reprints, *Critical points.

The chapter reviews the current state of knowledge of the thermodynamic behavior of fluids and fluid mixtures near the gas-liquid critical point. The concepts of simple, revised and extended scaling are explained, as they have evolved from the principle of critical point universality and the renormalization group approach. Critical point parameters and critical amplitudes are given for a dozen one component fluids, and revised and extended scaled formulations for five. The ranges of validity of these formulation and the problem of crossover to classical behavior are discussed. Several formulations of critical behavior, including their limitations, are described for fluid mixtures, and applications to vapor liquid phase equilibria, dilute mixtures and supercritical solubility are presented. The extrinsic and intrinsic effects of gravity on near critical fluids are described.

*600,589*
**PB87-13143**9 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Collision-Induced Radiative Transitions at Optical Frequencies.**
Final rept.,
P. S. Julienne. 1985, 22p
Pub. in Phenomena Induced by Intermolecular Interactions, p749-771 1985.

Keywords: Molecular spectroscopy, *Radiative collisions, *Atomic collisions, Optical frequency.

A brief overview is given in the field of collision-induced atomic radiative transitions at optical frequencies, including both collision-induced forbidden transitions and light induced collisional energy transfer (LICET). The main focus is on the theory of such processes. The theory of scattering in a radiation field can be used to calculate absorption or emission profiles, and the distribution of final product states. Several simplifying approximations greatly facilitate a qualitative understanding of the profile, but may fail in quantitative studies.

*600,590*
**PB87-131447** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Nonadiabatic Theory of Atomic Line Broadening: Final-State Distributions and the Polarization of Redistributed Radiation.**
Final rept.,
P. S. Julienne, and F. H. Mies. 1984, 13p
Pub. in Physical Review A: General Physics 30, n2 p831-843 Aug 84.

Keywords: Absorption, Reprints, *Line broadening, Electronic structure, Atom collisions.

The close coupled theory of atomic collisions in the presence of a radiation field may be used to calculate the distribution of final atomic states which results from absorption of polarized light during a collision. The theory applies equally well to optical collisions (line broadening) and to radiative collisions (laser induced collisional energy transfer). For an optical collision the detuning omega - omega (sub infinity) is restricted to be larger than either the Rabi frequency or the widths due to natural, Doppler, or pressure broadening. The radiation field is assumed to be weak enough that the transition probabilities are linear in field intensity. The molecular picture is emphasized in which the wavefunction is expanded in a basis of field-free molecular states and the Hamiltonian is blocked in accordance with molecular quantum numbers.

*600,591*
**PB87-131454** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Ab Initio Calculations of the Rotational Barriers in Formamide and Acetamide: The Effects of Polarization Functions and Correlation.**
Final rept.,
P. Jasien, W. Stevens, and M. Krauss. 1986, 10p
Pub. in Jnl. of Molecular Structure (Theochem) 139, p197-206 1986.

Keywords: *Acetamides, Molecular structure, Amides, Reprints, *Formamide, Rotational barriers.

Ab initio calculations have been used to determine the gas-phase rotational barrier about the CN bond in formamide and acetamide. The results indicate that the inclusion of polarization functions in the basis set leads to a substantial decrease (ca. 5 kcal/mol) in the calculated barrier height at the SCF level. Electron correlation effects decrease the barrier by less than 1 kcal/mol, while the addition of zero point energy corrections changes the barrier height only slightly. Based upon the current calculations, the 0 K rotational barriers for isolated formamide and acetamide are predicted to be 14.2 and 12.5 kcal/mol, respectively.

*600,592*
**PB87-131462** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Population Lifetimes of OH(v=1) and OD(v=1) Stretching Vibrations of Alcohols and Silanols in Dilute Solution.**
Final rept.,
E. J. Heilweil, M. P. Casassa, R. R. Cavanagh, and J. C. Stephenson. 1986, 15p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics 85, n9 p5004-5018, 1 Nov 86.

Keywords: *Molecular relaxation, Alcohols, Vibrations, Reprints, *Lifetime, Silanols, Picosecond pulses.

Picosecond infrared pump-probe experiments determined the vibrational population lifetimes (T1) of the hydroxyl fundamental stretching mode OH(nu = 1) in 12 alcohols (R3COH) and 8 silanols (R3SiOH) in dilute room temperature CCl solutions. T sub 1 for the silanols is in the range 185 < T sub 1 < 292 ps, while T sub 1 for the alcohols is much less (T sub 1 < 80 ps). The deuterium-exchanged analogs (COD and SiOD) exhibit population relaxation times similar to protonated hydroxyls. An analysis of the vibrational energy levels corresponding to modes involving the four bonds nearest the hydroxyl groups of these molecules is used to qualitatively explain the trends of the observed T sub 1 lifetimes for these systems. Solution T sub 1 lifetimes are also compared to those previously measured for OH (nu = 1) on the surface of silica and in other condensed phase, room temperature systems.

*600,593*
**PB87-131512** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of the Director.
**Comparison of Algorithms for X-ray Mass Absorption Coefficients.**
Final rept.,
K. F. J. Heinrich. 1986, 2p
Pub. in Microbeam Analysis-1986, p279-280.

Keywords: Algorithms, Absorption, Data reduction, Microanalysis, X-ray absorption, *Mass absorption coefficients, Electron probes.

A new model for the calculation of mass absorption coefficients is presented which takes into account the inaccuracy of the model mu = (C)(lambda sub n) used in the current algorithms for estimating mu, which are incorporated in data reduction programs for electron probe microanalysis.

*600,594*
**PB87-131827** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Simulation of Aerosol Agglomeration in the Free Molecular and Continuum Flow Regimes (Journal Version).**
Final rept.,
R. D. Mountain, G. W. Mulholland, and H. Baum. Nov 86, 15p
See also PB87-107777. Sponsored by Defense Nuclear Agency, Washington, DC.
Pub. in Jnl. of Colloid and Interface Science 114, n1 p67-81 Nov 86.

Keywords: *Aerosols, *Agglomeration, Colloids, Brownian movement, Soot, Reprints, Fractals.

The formation of high temperature aerosol agglomerates is simulated by following the Langevin trajectory of each particle with the boundary condition that the particles stick upon collision. Both the free molecular and continuum flow are treated. A new derivation of the friction force of an agglomerate in the continuum limit is developed based on the evaluation of the surface momentum flux at the Oseen flow limit. The agglomerates can be described as a fractal, at least in regard to the power law relationship between mass and size, with a dimensionality of 1.7-1.9 independent of the flow regime. The particle growth is shown to be much more rapid in the free molecular regime than in the continuum. The global kinetics are shown to be consistent with a similarity analysis of the coagulation equation with a modified coagulation coefficient. Comparison between the simulation and coagulation theory at small time suggests a slight fluctuation enhancement in the free molecule case and a small-time enhancement of the coagulation rate at high concentration for the continuum case.

*600,595*
**PB87-132064** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Enthalpy of Combustion of Purine.**
Final rept.,
D. R. Kirklin, and E. S. Domalski. 1984, 9p
Pub. in Jnl. of Chemical Thermodynamics 16, n7 p633-641 1984.

Keywords: *Combustion, *Enthalpy, *Purines, Thermodynamic properties, Chemical reactions, Nitrogen heterocyclic compounds, Heat of formation, Reprints.

The enthalpy of combustion for a commercial purine sample of better than 99 percent purity was measured in an aneroid adiabatic bomb calorimeter. The enthalpy of combustion at 298.15 K for the reaction, C5H4N4(c) + 6 O2(g) -> 5 CO2(g) + 2 H2O(l) + 2 N2(g) is delta(sub c) H = -(2708.63 + or - 2.23) kJ/mol. The corresponding enthalpy of formation for purine, C5H4N4, is delta(sub f) H = (169.42 + or - 2.26) kJ/mo1.

*600,596*
**PB87-132254** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**SIte Specificity in Stimulated Desorption from TiO2.**
Final rept.,
R. L. Kurtz, R. Stockbauer, and T. E. Madey. 1985, 5p
Pub. in Springer Ser. Surf. Sci. 4, p89-93 1985.

Keywords: *Surfaces, *Desorption, *Titanium dioxide, Chemisorption, Surface chemistry, Oxides, Reprints, Synchrotron radiation.

Synchrotron radiation has been combined with surface characterization techniques to study electron and photon-stimulated ion desorption from single-crystal TiO2. TiO2 is the model system for the Knotek-Feibelman mechanism describing the production and desorption of O(1+)-ions because it is a maximal-valent oxide: the Ti 3d-electron population on the stoichiometric, annealed surface is minimal. O-vacancy defects associated with appreciable Ti 3d-electron population can be created resulting in a non maximal-valent surface and straightforward interpretation of the Knotek-Feibelman mechanism would predict a reduced O(1+)-ion yield. Unexpected total ion-yield results have been obtained, however, and are shown to add new insights to the field of stimulated desorption.

*600,597*
**PB87-134177** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**HIgh Resolution IR Laser Spectroscopy of van der Waals Complexes in Slit Supersonic Jets: Observation and Analysis of nu(sub 1), nu(sub 1) + nu(sub 2), and nu(sub 1) + 2nu(sub 3) in ArHF.**
Final rept.,
C. M. Lovejoy, M. D. Schuder, and D. J. Nesbitt. 1986, 13p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 85, n9 p4890-4902, 1 Nov 86.

Keywords: Infrared spectroscopy, Supersonic aircraft, Jet aircraft, Reprints, *Van der Waals forces, Argon hydrogen fluorides, Tunable lasers.

IR spectra of jet cooled ArHF are obtained via direct absorption of a high resolution tunable difference frequency laser in a 2.54 cm path length, slit supersonic pulsed expansion at <10 K. Detection limits of 2x 10 to the 9th power molecules/cc/quantum state permit observation of the high frequency nu(sub 1) fundamental stretch (10(sup 0) 0) <- 00(sup 0) 0, the nu(sub 1) + nu(sub 2) van der Waals bend plus stretch combination band (11 (sup 1) 0) (00(sup 0) 0), as well as transitions to the 10(sup 0) 2 triply vibrationally excited state that are weakly allowed via Coriolis interactions with the Pi(sub 1+) component of the (11 (sup 1) 0) manifold. The ground state (00(sup 0) 0) molecular constants are in excellent agreement with previous microwave data.

*600,598*
**PB87-134201** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Ionisation of a One-Dimensional Hydrogen Atom by a Resonant Electric Field.**
Final rept.,
J. N. Bardsley, and M. J. Comella. 1986, 4p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 19, pL565-L568 1986.

Keywords: Excitation, Reprints, *Hydrogen atoms, *Multiphoton ionization, Rydberg states.

The complex coordinate method is used in quantum calculations of the rate of ionization of highly excited states of H atoms by microwave radiation. The results are compared with classical calculations by Leopold and Richards.

*600,599*
**PB87-134235** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Threshold Shift and Above-Threshold Multiphoton Ionization of Atomic Hydrogen in Intense Laser Fields.**
Final rept.,
S. I. Chu, and J. Cooper. 1985, 7p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC., and Department of Energy, Washington, DC.
Pub. in Physical Review A: General Physics 32, n5 p2769-2775 Nov 85.

Keywords: Ionization potentials, Reprints, *Hydrogen atoms, *Multiphoton ionization.

Accurate ab initio nonperturbative L(sup2) non-Hermitian Floquet calculations for intensity-dependent threshold shifts and ground-state total ionization widths (rates) for one-, two-, and three-photon-dominant intense-field ionization of atomic hydrogen are presented. The results show the importance of both the ac Stark shift and the pondermotive potential in the determination of the net threshold shift. In addition, branching ratios to individual continua have been estimated, yielding physical insights regarding the general features and mechanisms of the frequency- and intensity-dependent continuum-continuum transitions and 'peak switching' phenomena in the above-threshold ionization processes.

*600,600*
**PB87-134250** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Silane Discharge Gas and Surface Reactions.**
Final rept.,
A. Gallagher. 1985, 12p
Pub. in Proceedings of Symposium on Plasma Synthesis and Etching of Electronic Materials, Boston, MA., November 27-30, 1984, v38 p99-110 1985.

Keywords: *Silanes, Discharge, Chemical radicals, *Surface reactions.

Ion chemistry and neutral radical chemistry in silane discharges are described. A method by which the dominant SiH3 radical produces surface growth is suggested, and surface reactions are suggested as the principal source of Si2Hn species.

*600,601*
**PB87-134268** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Preparation and Detection of Alignment with High /m/ Selectivity by Saturated Laser Optical Pumping in Molecular Beams.**
Final rept.,
U. Hefter, G. Ziegler, A. Mattheus, A. Fischer, and K. Bergmann. 1986, 17p
Pub. in Jnl. of Chemical Physics 85, n1 p286-302, 1 Jul 86.

Keywords: Atomic energy levels, Orientation, Neon, Sodium, Reprints, *Molecule-molecule collisions, Optical pumping, Molecular beams.

The authors describe a technique for preparation of molecules in single /m/ levels involving saturated laser optical pumping on molecular P, R, and Q transitions. The technique is not limited to small rotational quantum numbers j. It allows the determination of the populations of /m/ levels for arbitrary distribution functions f(j,m) or alternatively, the determination of all moments of f(j,m). In principle, the method is able to completely determine the angular distribution of j vectors. Experimental verification of the high /m/-state purity achieved in Na2 supersonic beams, as well as of inherent limitations due to hyperfine interaction is provided. For illustration, experimental data on laser-induced alignment, the dependence of the flow induced molecular alignment, and on delta m-propensity rules in differential rotationally inelastic scattering are presented.

*600,602*
**PB87-134284** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Rational Approximations for the Holtsmark Distribution, Its Cumulative and Derivative.**
Final rept.,
D. G. Hummer. 1986, 5p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 36, n1 p1-5 1986.

Keywords: *Quantum chemistry, Approximation, Reprints, Holtsmark distribution.

The convergent series expansions of the Holtsmark distribution P(beta), its cumulative Q(beta), its derivative R(beta) and the semiconvergent asymptotic series for these functions are used to calculate rational approximations for P,Q, and R, which are valid for all positive beta and have maximum errors of approximately 10 to the 8th power, 10 to the 9th power, 10 to the 7th power, respectively.

*600,603*
**PB87-134870** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Observation of the 3s (sup 2)A(sub 1) Rydberg States of Allyl and 2-Methylallyl Radicals with Multiphoton Ionization Spectroscopy.**
Final rept.,
J. W. Hudgens, and C. S. Dulcey. 1985, 5p
Pub. in Jnl. of Physical Chemistry 89, n8 p1505-1509 1985.

Keywords: *Chemical radicals, Excitation, Absorption, Reprints, *Chemical reaction kinetics, *Rydberg states, Multiphoton ionization, Allyl radicals, Methylallyl radicals.

Previously unreported bands of allyl, allyl-d, and 2-methylallyl radicals have been detected by mass resolved resonance enhanced multiphoton ionization spectrometry. Focused laser light between 480-535 nm induced two photon absorptions preparing the 3s (sup 2) A (sub 1) Rydberg states of the radicals. Absorption of two additional photons ionized the excited radicals. These electronic states of allyl and 2-methylallyl radicals lie at 40085/cm and 38369/cm respectively. No subsequent fragmentation of the molecular ions was observed.

*600,604*
**PB87-134912** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**New Efficient Far Infrared Lasing Molecule: (13)CD3OH.**
Final rept.,
M. Inguscio, K. M. Evenson, F. R. Petersen, F. Strumia, and E. Vasconcellos. 1984, 8p
Pub. in International Jnl. of Infrared and Millimeter Waves 5, n9 p1289-1296 1984.

Keywords: Deuterated compounds, Frequency measurement, Far infrared radiation, Infrared lasers, Reprints, *Methyl alcohol isotopic species.

Thirty-six new cw laser lines ranging from 52 to 469 micrometers are obtained by pumping, for the first time, the isotope of methyl alcohol (13)CD3OH. The new laser line at 127.0 micrometers is one with the highest efficiency ever reported. Direct frequency measurements are reported for eleven new lines.

*600,605*
**PB87-134946** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Laboratory Measurement of the Rotational Spectrum of the OH Radical with Tunable Far-Infrared Radiation.**
Final rept.,
J. M. Brown, L. R. Zink, D. A. Jennings, K. M. Evenson, and A. Hinz. 1986, 4p
Sponsored by National Aeronautics and Space Administration, Washington, DC., and Chemical Manufacturers Association, Washington, DC.
Pub. in Astrophysical Jnl. 307, p410-413, 1 Aug 86.

Keywords: *Rotational spectra, Far infrared radiation, Frequency measurement, Reprints, *Hydroxyl radicals, Tunable lasers.

Rotational and fine-structure transitions between the low rotational levels of the OH radical in its X (sup 2) Pi state have been observed in absorption in the laboratory. It has thus been possible to measure the frequencies of these transitions directly. The observations were made with tunable far-infrared radiation generated by mixing two chosen CO2 laser frequencies in a metal-insulator-metal diode; the far-infrared difference frequency was radiated from the diode's whisker antenna. The measurements have an accuracy of a few hundred kHz. They both confirm and improve on the best previous estimates, which were obtained by extrapolation of laser magnetic resonance data.

*600,606*
**PB87-134961** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Thermodynamic Anomalies in Near-Critical Aqueous NaCl Solutions.**
Final rept.,
J. M. H. Levelt Sengers, C. M. Everhart, G. Morrison, and K. S. Pitzer. 1986, 14p
Pub. in Chemical Engineering Communications 47, p315-328 1986.

Keywords: *Sodium chloride, Thermophysical properties, Solutions, Abnormalities, Reprints.

Apparent molar properties of near-critical aqueous NaCl solutions have been reported to show very large anomalies. The authors show that these anomalies are to be expected in any dilute solution of a nonvolatile in a near-critical solvent. Debye-Huckel effects need to be handled with some care; if inserted in the Helmholtz free energy, they cause no more than a higher-order effect.

*600,607*
**PB87-134979** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Dilute Mixtures and Solutions Near Critical Points.**
Final rept.,
J. M. H. Levelt Sengers. 1986, 9p
Pub. in Fluid Phase Equilibria 30, p31-39 1986.

Keywords: Thermophysical properties, Equilibrium, Fluid dynamics, Impurities, Reprints, *Critical fluids.

At given pressure and temperature, impurities have very large effects on the density and enthalpy of near-critical fluids because the derivative (partial derivative of V with respect to x)(sub PT) diverges. Thermodynamic relations permit to calculate impurity effects from the initial slope of the critical line or from the dew-bubble curve. Examples are given for both nonaqueous and aqueous mixtures.

*600,608*
**PB87-134987** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Molecular Dynamics Study of Compositional Order in a Binary Fluid Mixture.**
Final rept.,
R. D. Mountain. 1986, 11p
Pub. in Molecular Physics 59, n4 p857-867 1986.

Keywords: Liquids, Reprints, *Molecular dynamics, *Binary mixtures.

Molecular dynamics is used to investigate the connection between strong compositional order in a binary liquid mixture and the interactions between the unlike species of the mixture. Two classes of models are examined. The first has strong attraction between the unlike species and the second has purely repulsive interactions with a nonadditive diameter for the unlike pairs which is less than the average of the diameters of the like pairs. Both models lead to compositional ordering. The structure is characterized in terms of both pair and three-particle correlation functions which are constructed during the molecular dynamics computations. The connection of these models with observations of compositional ordering in alloys is discussed. Also, the possible utility of purely repulsive models for characterizing a wide range of binary liquid mixture properties is mentioned.

*600,609*
**PB87-135026** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Molecular Beam Study of Electronic to Electronic, Vibrational, and Rotational Energy Transfer in the Collision of Two Step Laser Excited Sodium with N2.**
Final rept.,
G. Jamieson, W. Reiland, C. P. Schulz, H. U. Tittes, and I. V. Hertel. 1984, 6p
Pub. in Jnl. of Chemical Physics 81, n12 p5805-5810 1984.

Keywords: *Nitrogen, Excitation, Quenching, Atomic energy levels, Reprints, *Sodium atoms, *Atom-molecule collisions.

The quenching of excited Na(sup *)(4d/5s,4p,4s) by N2 has been studied in a crossed atomic and molecular beam apparatus at thermal collision energies. The sodium atoms are excited by two laser beams of different wavelengths to either the 4 doublet S(sub 1/2) or 5 doublet S(sub 1/2) state, via the intermediate 3 doublet P(sub 3/2) state. For both excitation schemes optical relaxation processes lead to a population in the 4 doublet P(sub 3/2) and 4 doublet S(sub 1/2) states of several percent. The relative densities of the excited states have been calculated from rate equations using stationary conditions. The structure can be partially disentangled using the results of the previously studied Na(sup *) (3 doublet P(sub 3/2)) + N2 quenching process. The main conclusion is that collisional deexcitation to the Na(3s) ground state is negligible whereas among the higher levels the collisional energy transfer cross sections are between 0.5 and 7.5 times the magnitude of the 3p-3s quenching cross section and they are strongly forward peaked in the same way.

*600,610*
**PB87-135232** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Comparison of the Ground State Vibrational Fundamentals of Diatomic Molecules in the Gas Phase and in Inert Solid Matrixes.**
Final rept.,
M. E. Jacox. 1985, 16p
Pub. in Jnl. of Molecular Spectroscopy 113, n2 p286-301 1985.

Keywords: *Molecular structure, Ground state, Vibrational spectra, Reprints, *Diatomic molecules, Van der Waals forces, Charge transfer.

Despite the voluminous literature on the spectra of diatomic molecules, there are many gaps in the knowledge of the ground-state vibrational frequencies. For many important diatomic molecules, only values obtained in matrix isolation experiments are available. In order to assess the likely extent of deviation of the ground-state deltaG(1/2) values of diatomic molecules observed in rare-gas and nitrogen matrices from the gas-phase values, a systematic comparison has been made between gas-phase and matrix frequencies. The dependence of matrix shifts on the matrix material and type of chemical bond is considered for the approximately 230 pairs of observations, spanning the entire Periodic Table, which have been reported. Except for van der Waals molecules and for the Group Ia and IIIa halides, the argon-matrix shift for most diatomic molecules is less than 2%.

*600,611*
**PB87-136594** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Vibrational Relaxation of HCl in Dilute CCl4 and CCl3F Solutions.**
Final rept.,
J. T. Knudtson, and J. C. Stephenson. 1984, 4p
Pub. in Chemical Physics Letters 107, n4-5 p385-388 1984.

Keywords: *Carbon tetrachloride, *Molecular relaxation, Molecular spectroscopy, Reprints, *Methane/fluoro-trichloro, Chlorofluorocarbons, Picosecond pulses.

Picosecond infrared pump, spontaneous anti-Stokes Raman probe experiments determined the vibrational relaxation rates of HCl(v=1) dilute in liquid CCl4 and CCl3F at T=295 K to be 2.12(+ or - .14) x 10 to the 8th power /s and 1.57( + or - .22) x 10 to the 8th power/s, respectively. If the liquid phase data are interpreted in terms of the isolated binary collision model, the resultant deactivation probabilities are consistent with an extrapolation of gas phase results.

*600,612*
**PB87-136602** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Relativistic Effective Potential SCF Calculations of AgH and AuH.**
Final rept.,
M. Krauss, W. J. Stevens, and H. Basch. 1985, 9p
Pub. in Jnl. of Computational Chemistry 6, n4 p287-295 1985.

Keywords: Hydrides, Dipole moments, Reprints, *Hydride/silver, *Hydride/gold, Relativistic effective potentials.

Relativistic effective potential (REP) are now widely used in molecular electronic structure calculations. Tests of these REP are needed to assess their accuracy. This can now be done for AgH and AuH since Lee and McLean have published Dirac-Fock calculations for these molecules. Comparative SCF calculations have been performed for two types of effective potential. Satisfactory agreement between the effective potential results for spectroscopic constants and dipole moments with the Dirac-Fock values is found which supports the use of these potentials for heavy atom containing molecules.

*600,613*
**PB87-136669** PC **A16**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.
**Technical Activities 1986, Center for Chemical Physics,**
P. Ausloos. Oct 86, 366p NBSIR-86-3470
See also PB86-157336.

Keywords: *Research projects, Molecular spectroscopy, Surface chemistry, Reaction kinetics, Thermodynamics, *Chemical physics.

The report summarizes research projects, measurement method development, testing and data evaluation activities carried out during Fiscal Year 1986 in the NBS Center for Chemical Physics. These activities fall in the areas of surface science, chemical kinetics, chemical thermodynamics and molecular spectroscopy.

*600,614*
**PB87-137188**
(Order as PB87-137154, PC **A04**/MF **A01**)
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Thermal Expansion of Platinum and Platinum-Rhodium Alloys,**
R. E. Edsinger, M. L. Reilly, and J. F. Schooley. 23 Jul 86, 23p
Included in Jnl. of Research of the National Bureau of Standards, v91 n6 p333-362 Nov-Dec 86.

Keywords: *Thermal expansion, *Platinum, Thermodynamic properties, *Platinum rhodium alloys.

The paper contains descriptions of the construction and use over the temperature range -27C to 570C of a Merritt-Saunders (optical interferometric) linear thermal expansion apparatus. Measurements of thermal expansion are reported for platinum and for two platinum-rhodium alloys (nominally 12 wt% Rh and 20 wt% Rh). Detailed analyses are given of the measurement uncertainties involved in the experiment and of the representation of the data by polynomials in the sample temperatures. The data show precision at the 1-ppm level and good agreement with results already published.

*600,615*
**PB87-140570** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Center for Chemical Engineering.
**Computer Code for Gas-Liquid Two-Phase Vortex Motions: GLVM,**
T. T. Yeh. Jul 86, 45p NBSIR-86/3414
Sponsored by National Aeronautics and Space Administration, Cocoa Beach, FL. John F. Kennedy Space Center.

Keywords: *Liquid phases, Mathematical models, Vortices, *Vortex separation process, *Vapor phases, Computer applications.

A computer program aimed at the phase separation between gas and liquid at zero gravity, induced by vortex motion, is developed. It utilizes an explicit solution method for a set of equations describing rotating gas-liquid flows. The vortex motion is established by a tangential fluid injection. A Lax-Wendroff two-step (McCormack's) numerical scheme is used. The program can be used to study the fluid dynamical behavior of the rotational two-phase fluids in a cylindrical tank. It provides a quick/easy sensitivity test on various parameters and thus provides the guidance for the design and use of actual physical systems for handling two-phase fluids.

*600,616*
**PB87-145066** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.

**Interactive FORTRAN Programs for Micro Computers to Calculate the Thermophysical Properties of Twelve Fluids (MIPROPS).**
Technical note,
R. D. McCarty. May 86, 92p NBS/TN-1097
Also available from Supt. of Docs as SN003-003-02745-6. Sponsored by National Aeronautics and Space Administration, Houston, TX. Lyndon B. Johnson Space Center.

Keywords: *Thermophysical properties, *Transport properties, *Helium, *Hydrogen, *Nitrogen, *Oxygen, *Methane, *Ethylene, *Propane, *Butanes, *Argon, *Liquid helium, *Liquefied gases, Viscosity, Density, Fluids, Computer programs, Entropy, Enthalpy, Thermal conductivity, Vapor phases, Nitrogen fluorides, *Nitrogen fluoride(NF3), Fortran 77 programming language, Dielectric constant, Heat capacity.

The thermophysical and transport properties of selected fluids have been programmed in FORTRAN 77 which is available for micro computers. The input variables are any two of P, p, T (pressure, density, and temperature) in the single phase regions, and either P or T for the saturated liquid or vapor states. The output is pressure, density, temperature, internal energy, enthalpy, entropy, specific heat capacities (C(sub p) and C(sub v)), speed of sound and, in most cases, viscosity, thermal conductivity, and dielectric constant. The fluids included are: helium, hydrogen, nitrogen, oxygen, argon, nitrogen trifluoride, methane, ethylene, ethane, propane, iso- and normal butane. The programs give properties in both the liquid and vapor states over a wide range of temperature and pressure. Copies of the program may be obtained from the Office of Standard Reference Data, Room A320, Physics Building, National Bureau of Standards, Gaithersburg, MD 20899.

*600,617*
**PB87-145371** Not available NTIS
American Chemical Society, Washington, DC.
**Journal of Physical and Chemical Reference Data, Volume 14, 1985, Supplement No. 1. JANAF Thermochemical Tables, 3rd Edition, Parts 1 and 2.**
M. W. Chase, C. A. Davies, J. R. Downey, D. J. Frurip, and A. N. Syverud. c1986, 1880p
Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermochemical properties, Tables(Data), Thermodynamic properties, Specific heat, Entropy, Enthalpy, Gibbs free energy, Temperature.

Recommended temperature-dependent values are provided for chemical thermodynamic properties of inorganic substances and for organic substances containing only one or two carbon atoms. These tables cover the thermodynamic properties over a wide temperature range with single-phase and multiphase tables for the crystal, liquid, and ideal gas state. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states. All values are given in SI units and are for a standard-state pressure of 100,000 Pa (1 bar). Each tabulation is accompanied by a critical evaluation of the literature upon which the thermochemical table is based. Literature references are given. The volume is a new collective edition of five previous publications. In it all tabulations have been rewritten in a consistent style. Many, but not all, tabulations have been revised as a result of a reevaluation of the data. (Copyright (c) 1986 by the U.S. Secretary of Commerce on behalf of the United States. This copyright will be assigned to the American Insitute of Physics and the American Chemical Society, to whom all requests regarding reproduction should be addressed).

*600,618*
**PB87-148300** Not available NTIS
American Chemical Society, Washington, DC.
**Journal of Physical and Chemical Reference Data, Volume 15, Number 4, 1986.**
Quarterly rept.
c1986, 196p
See also PB87-148318 through PB87-148375, and PB87-109963. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research, Water, Viscosity, Thermal conductivity, Transport properties, Hydrogen, Argon, Thermodynamic properties, Alkyne compounds, Deuterium, Actinide series compounds, Oxygen organic compounds, Triple point, Rate constants.

Topics include: Improved international formulations for the viscosity and thermal conductivity of water substance; The viscosity and thermal conductivity of normal hydrogen in the limit of zero density; The viscosity and thermal conductivity coefficients of gaseous and liquid argon; Standard chemical thermodynamic properties of alkyne isomer groups; Recent progress in deuterium triple-poimt measurements; Rate constants for reactions of radiation-produced transients in aqueous solutions of actinides; Thermodynamic properties of key organic oxygen compounds in the carbon range C1 to C4. Part 2. Ideal gas properties.

*600,619*
**PB87-148318** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Improved International Formulations for the Viscosity and Thermal Conductivity of Water Substance,**
J. V. Sengers, and J. T. R. Watson. c1986, 24p
Prepared in cooperation with National Engineering Lab., East Kilbride (Scotland).
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1291-1314 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Water, *Viscosity, *Thermal conductivity, Transport properties, Tables(Data).

The paper describes improved international formulations for the viscoisity and thermal conductivity of water substance recently adopted by the International Association for the Properties of Steam.

*600,620*
**PB87-148326** Not available NTIS
Thessaloniki Univ., Salonika (Greece). Dept. of Chemical Engineering.
**Viscosity and Thermal Conductivity of Normal Hydrogen in the Limit of Zero Density,**
M. J. Assael, S. Mixafendi, and W. A. Wakeham. c1986, 8p
Prepared in cooperation with Imperial Coll. of Science and Technology, London (England). Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1315-1322 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Hydrogen, *Thermal conductivity, *Viscosity, Gases, Temperature dependence.

The paper contains a new representation of the viscosity and thermal conductivity coefficients of normal hydrogen in the limit of zero density as a function of temperature. The correlation is based upon the semiclassical kinetic theory of polyatomic gases and a body of critically evaluated experimental data. In the temperature range 200-400 K the accuracy of the representation of the viscosity is estimated to be plus or minus 0.5%. However, at the lowest temperature of 20 K and the highest temperature of 2200 K, the uncertainty rises to plus or minus 2.0%. The available thermal conductivity data of high accuracy cover the much more restricted temperature range from 100 to 400 K and the correlation of this property is limited to that range. An attempt has also been made to represent the viscosity data by means of a correlation universal among several other polyatomic gases but it has proven unsatisfactory.

*600,621*
**PB87-148334** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Viscosity and Thermal Conductivity Coefficients of Gaseous and Liquid Argon,**
B. A. Younglove, and H. J. M. Hanley. c1986, 16p
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1323-1337 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Argon, *Viscosity, *Thermal conductivity, Thermophysical properties, Gases, Liquids.

Data for the viscosity and thermal conductivity of gaseous and liquid argon have been evaluated and represented by empirical functions. Tables for the viscosity from 86 to 500 K for pressures to 400 MPa, and for the thermal conductivity from 90 to 500 K for pressures to 200 MPa are presented. For the viscosity, uncertainties of 2% or better for pressures below 100 MPa, and 3% for higher pressures are assigned. For the thermal conductiviy the uncertainties are 4% for temperatures below 150 K and 3% or better for temperatures above. The enhancement in the conductivity close to the critical point has been accounted for. The status of the argon transport data and the philosophy of fitting them are reviewed.

*600,622*
**PB87-148342** Not available NTIS
Massachusetts Inst. of Tech., Cambridge. Dept. of Chemistry.
**Standard Chemical Thermodynamic Properties of Alkyne Isomer Groups,**
R. A. Alberty, and E. Burmenko. c1986, 12p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1339-1347 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermodynamic properties, *Alkyne compounds, Enthalpy, Entropy, Gibbs free energy, Specific heat.

The chemical thermodynamic properties of alkyne isomer groups from C2H2 to C5H8 in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of C6H10 to C8H14 have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. for isomer group properties, increments per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Values of C(sub p),S, delta(sub f) H, and delta(sub f) G are given for all species from C2H2 to C8H14 in SI units for a standard state pressure of 1 bar.

*600,623*
**PB87-148359** Not available NTIS
Los Alamos National Lab., NM.
**Recent Progress in Deuterium Triple-Point Measurements,**
L. A. Schwalbe. c1986, 6p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1351-1356 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Deuterium, Hydrogen isotopes, *Triple point.

The triple point of deuterium is a proposed reference for defining the temperature scale between 13.81 and 24.562 K. The author reviewed recent measurements of this fixed point; the discussion concentrates on experiments with samples confined in transportable sealed cells. The authors also present theoretical estimates of the dependence of the triple-point temperature on the spin composition of the sample. Satisfactory agreement is obtained with experimental data on deuterium at low concentrations of the para (J=1) species. Present results support the adoption of the triple point of e-D(sub 2) as a standard temperature reference.

*600,624*
**PB87-148375** Not available NTIS
Texas A and M Univ., College Station. Thermodynamics Research Center.
**Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C1 to C4. Part 2. Ideal Gas Properties,**
J. Chao, K. R. Hall, K. N. Marsh, and R. C. Wilhoit. c1986, 68p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v15 n4 p1369-1436 1986. Available from Ameri-

can Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermodynamic properties, *Oxygen organic compounds, Specific heat, Enthalpy, Ideal gas.

The ideal gas thermodynamic properties of forty-four key organic oxygen compounds in the carbon range C1 to C4 have been calculated by a statistical mechanical technique. The properties determined are the heat capacity, entropy, enthalpy, and Gibbs energy function. The calculations have been performed, in most cases, over the temperature range 0 to 1500 K and at 1 bar. The contributions to the thermodyamic properties of compounds having internal-or-pseudo-rotations have been computed by employing a partition function formed by the summation of the internal rotational or pseudorotational energy level for each rotor in the given molecule. These energy levels have been calculated by solving the wave equation using appropriate barrier heights, rotational constants, and potential functions for the given rotations. The thermodynamic properties have been calculated using a rigid-rotor and harmonic-oscillator molecular model for each species.

## Polymer Chemistry

*600,625*
**PATENT-4 536 523** Not available NTIS
Department of Health and Human Services, Washington, DC.
**Dental Composite Formulation from Acrylate Monomer and Polythiol Accelerator.**
Patent,
J. M. Antonucci. Filed 23 Dec 83, patented 20 Aug 85, 6p PB86-218989, PAT-APPL-6-565 212
Supersedes PB84-159946.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Patents, *Dental materials, *Acrylate copolymers, *Synthesis(Chemistry), *Polymerization, Storage, Stability, Discoloration, Monomers.

A two paste dental composite formulation is disclosed, wherein one paste comprises a polymerizable monomer and a stable organic hydroperoxide initiator, and the other paste comprises a polymerizable monomer and a polythiol accelerator, the hydroperoxide having a ten-hour half-life temperature in excess of about 100 degrees C., and the polythiol being capable of accelerating the decomposition of the hydroperoxide into polymerization initiating free radicals at ambient temperatures.

*600,626*
**PB86-185485** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Small-Angle Neutron Scattering of Partially Segregated Amorphous Polyethylene Terephthalate.**
Final rept.,
W. Wu, D. Wiswe, H. G. Zachmann, and K. Hahn. 1985, 6p
Sponsored by Hamburg Univ. (Germany, F.R.).
Pub. in Polymer 26, n5 p655-660 1985.

Keywords: *Polyethylene terephthalate, Deuterium compounds, Neutron scattering, Reprints, Small angle scattering, Amorphous materials.

Deuterated polyethylene terephthalate (DPET) was synthesized from deuterated ethylene glycol and deuterated dimethyl terephalate which was derived from 1,4-dibromobenzene. Amorphous specimens for the small angle neutron scattering (SANS) were prepared by solution blending the DPET with the hydrogenerated PET and subsequently melt pressing. The SANS results suggested the occurrence of both segregation and transesterification between the deuterated and hydrogenerated species. An expression for the scattered intensities from partially segregated blends has been derived. Using this expression the average molecular weight, radius of gyration as well as the size of the segregation domains can be determined quantitatively from the SANS data.

*600,627*
**PB86-192788** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Molecular Weight Effects on the Phase Diagram of Polystyrene-Poly(vinyl methyl ether) Blends.**
Final rept.,
J. M. Ubrich, F. B. C. Larbi, J. L. Halary, L. Monnerie, and B. J. Bauer. 1986, 7p
Pub. in Macromolecules 19, n3 p810-815 1986.

Keywords: *Molecular weight, *Polystyrene, *Polyrinyl methyl ether, Phase diagrams, Vinyl ether resins, Reprints.

Fluorescence emission of labeled polystyrene is employed to reexamine the lower critical solution temperature phase diagram of the system polystyrene (PS)-poly(vinyl methyl ether) (PVME) over a large range of molecular weights. The influence of polymer chain length is investigated by using a variety of PS's and PVME's having molecular weights ranging from 20 400 to 1660 000 and from 45 000 to 1330 000, respectively. Fluorescence measurements are shown to be suitable for the determination of the coexistence curve, even in the case of the largest molecular weights, for which the phase separation process develops very slowly. Particular attention is paid to a series of blends in which the molecular weight of one component is kept constant, whereas that, M(sub w)(i), of the other one varies.

*600,628*
**PB86-192952** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Anomalies in the Physical Ageing Behavior of PMMA.**
Final rept.,
G. B. McKenna, and A. J. Kovacs. 1983, 2p
Sponsored by Centre National de la Recherche Scientifique, Strasbourg (France). Centre de Recherches sur les Macromolecules.
Pub. in Polym. Prepr. 24, n2 p100-101 1983.

Keywords: *Polymethyl methacrylate, Aging tests(Materials), Stress relaxation, Torque, Deformation, Cylinders, Reprints.

Cylindrical specimens of PMMA were quenched from above the glass transition and subsequently tested in torsion. Torque and normal force relaxation responses were recorded. The experiments were performed at 40 deg, 60 deg and 80 deg C and at increasing ageing times. Two anomalies from the classical picture of ageing were revealed by these investigations: (1) The small deformation relaxation curves could not be superposed by any combination of vertical and horizontal shifts. (2) The ageing responses of the torque relaxation and normal force relaxation at mode-rate deformations (gamma approx. 0.04), while superposeable, are different. The shift required to superpose the normal force response is two times that required to superpose the torque response.

*600,629*
**PB86-193539** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Polymeric Electrolyte Based on Poly(ethylene imine) and Lithium Salts.**
Final rept.,
C. K. Chiang, G. T. Davis, C. A. Harding, and T. Takahashi. 1986, 6p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Solid State Ionics 18 and 19, p300-305 1986.

Keywords: *Batteries, *Conductivity, Ionic conduction, Lithium salts, Electrolytes, Polymers, Reprints, Poly(ethylene imine).

The dissolution of lithium salts in linear poly(ethylene imine) has been investigated because of its possible role as a solid electrolyte in lithium batteries. Lithium salts included in the study are LiF, LiCl, LiBr, LiI, LiSCN, LiC104 and LiBF4. When cast from solution in a common solvent, a uniform mixture is obtained (except for the case of LiF). Interaction of the salt and polymer can be characterized by observing a loss in crystallinity of the polymer and an increase in the glass transition temperature. At concentrations of salt below 10 mole percent, the polymer can slowly recrystallize at room temperature but at higher concentrations, the mixture remains amorphous for an indefinite period of time. DC conductivity at room temperature is about 1 times 10 to the 8th power S/cm but increases to 0.0001 S/cm at 150 C.

*600,630*
**PB86-193612** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Laser Ionization Mass Spectrometry of Poly(4-vinylpyridine).**
Final rept.,
R. A. Fletcher, and A. J. Fatiadi. 1985, 3p
Pub. in Polymer Communications 26, p270-272 Sep 85.

Keywords: Mass spectroscopy, Reprints, *Laser enhanced ionization, *Poly(ethylene/pyridyl).

Commercial poly(4-vinylpyridine) (PVP) solid beads have been investigated by laser ionization mass spectrometry using a Laser Microprobe Mass Analyzer (LAMMA 500). The objective was to structurally characterize the fragment ion patterns of both the positive and negative ion mass spectra. Main emphasis is placed on PVP 2% crosslinked with divinylbenzene, but comparison with non-crosslinked PVP and 25% crosslinked samples as well as HCl treated 2% crosslinked PVP are reported.

*600,631*
**PB86-193703** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Chemical Modification of Poly(ethylene imine) for Polymeric Electrolyte,**
Final rept.,
T. Takahashi, G. T. Davis, C. K. Chiang, and C. A. Harding. 1986, 5p
See also AD-A160 482. Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Solid State Ionics 18 and 19, p321-325 1986.

Keywords: Ionic conduction, Electrolytes, Reprints, *Conductivity, *Cross linking.

Linear PEI has been chemically modified in an attempt to prevent formation of a crystalline complex without altering its ability to dissolve salts and conduct ions. Three main systems were investigated: (a) poly(N-acetylethylene imine), (b) partially quaternized PEI with ethyl or butyl groups, and (c) PEI cross-linked with diepoxyoctane. Dissolution of salt was followed by x-ray diffraction on the mixtures and changes in Tg as determined by DSC. In all cases, the crystallinity was destroyed but conductivity of salt-containing polymer was not improved. However, lightly cross-linked PEI exhibits much improved mechanical properties and the incorporation of .05 mole NaI/mole of monomer yields a conductivity of 5 times 10 to the 5th power S/cm at 100 C.

*600,632*
**PB86-193737** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Equilibrium Phase Compositions of Heterogeneous Copolymers.**
Final rept.,
B. J. Bauer. 1985, 7p
Pub. in Polymer Engineering and Science 25, n17 p1081-1087 Dec 85.

Keywords: *Copolymers, *Polymerization, Thermodynamic properties, Phase diagram, Heterogeneity, Reprints.

The products of random copolymerizations are heterogeneous in chemical composition, having a distribution of the fraction of each monomer in the copolymer. Polymer molecules with the same composition and molecular weight can be treated as separate components in a polymer blend. The spinodal limit is a simple function of chemical heterogeneity. The equilibrium number of phases, phase volumes, and average composition can be calculated from the condition that the chemical potential of a polymer species is equal in every phase. Phase diagrams are calculated for various hypothetical chemical distributions as well as a distribution characteristic of a random acrylonitrilebutadiene copolymerization to high conversion.

*600,633*
**PB86-195773** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

**Picosecond Excimer Fluorescence Spectroscopy: Applications to Local Motions of Polymers and Polymerization Monitoring.**
Final rept.,
F. W. Wang, R. E. Lowry, and R. R. Cavanagh. 1985, 5p
Contract ARO-111-84
Sponsored by Army Research Office, Research Triangle Park, NC.
Pub. in Polymer 26, p1657-1661 1985.

Keywords: *Energy migration, Methyl methacrylate, Monitoring, Spectroscopy, Polymerization, Reprints, *Excimer fluorescence.

The local motions of bis-(1-pyrene)alkanes and pyrene-labelled poly(methyl methacrylate) polymers in solution were characterized by picosecond excimer fluorescence spectroscopy. The experimental results showed that 1,3-bis-(1-pyrene)propane and 1,10-bis-(1-pyrene)decane have similar local motions that bring two pyrene groups together to form excimers. Further, poly(1-pyrenylmethyl methacrylate) and a copolymer of methyl methacrylate and 1-pyrenylmethyl methacrylate in solution were found to have similar local motions that lead to excimer formation. In addition, the viscosity change during the polymerization of methyl methacrylate was monitored by measuring with picosecond fluorimetry the fluorescence lifetime of a trace amount of 1,3-bis-(1-pyrene)propane dissolved in methyl methacrylate.

*600,634*
**PB86-195781** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Self-Diffusion in Concentrated Polystyrene Solutions Measured by Fluorescence Recovery After Photobleaching.**
Final rept.,
F. W. Wang, R. E. Lowry, and E. S. Wu. 1985, 3p
Pub. in Polymer 26, p1654-1656 1985.

Keywords: *Esterification, Polystyrenes, Reduction, Reprints, *Carboxylation, Photobleaching.

A polystyrene polymer of narrow molecular weight distribution was carboxylated, then reduced, and finally esterified with NBD-aminohexanoic acid (6-(7-nitrobenz-2-oxa-1,3-diazol-4-yl)-aminohexanoic acid). The self-diffusion of the NBD-labelled polystyrene polymer in concentrated solutions of the unlabelled polystyrene polymer was measured by the method of fluorescence recovery after photobleaching over a concentration range from 0.017 g/ml to 0.41 g/ml at room temperature. In the semi-dilute region, the concentration dependence of diffusion coefficient was found to be in agreement with the predictions of scaling concepts.

*600,635*
**PB86-208469** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Structure of Metal-Coordinated Polymers: Laser Desorption of Poly(4-Vinylpyridine) and Poly(4-Vinylpyridine)-Metal Complexes.**
Final rept.,
R. A. Fletcher, and A. J. Fatiadi. 1984, 1p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Army Materials and Mechanics Research Center, Watertown, MA.
Pub. in Proceedings of Annual Conference on Microbeam Analysis Society (19th), Bethlehem, PA., July 16-20, 1984, Microbeam Analysis-1984, p14.

Keywords: *Polymers, *Metals, Lasers, Desorption, *Poly(4-vinylpyridine).

No abstract available.

*600,636*
**PB86-231495** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Assignment of IR (Infra-Red) Band Near 680/cm in Polyethylene to Molecular Twist Boundaries,**
D. H. Reneker, J. Mazur, and B. M. Fanconi. Nov 85, 3p
Pub. in Polymer Communications 26, p332-334 Nov 85.

Keywords: *Polyethylene, *Molecular structure, Polymers, Infrared spectra, Crystal defects, Reprints.

An infra-red absorption band in polyethylene near 680/cm is assigned to a rocking mode vibration of a twisted segment of a polyethylene zig-zag on the basis of calculations of the vibrational modes of defects in crystalline polyethylene in their minimum energy conformations. The twisted segments are probably associated with twist boundaries.

*600,637*
**PB87-105151** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
**Polymer Science Standards Division.**
Final rept.,
R. K. Eby. 1982, 5p
Pub. in Kobunshi/High Polymers Japan 31, p1026-1030 1982.

Keywords: *Polymers, Projects, History, Research, Reprints, National Bureau of Standards.

The article (in Japanese) was prepared at the invitation of the Society of Polymer Science (Japan) for publication in its Official Bulletin, KOBUNSHI/High Polymer Science Japan. There has been research on polymeric materials since the early days of the United States National Bureau of Standards. The background and function of the Polymer Science and Standards Division is reviewed. The present program is discussed in the context of the large, rapidly growing, and economically important U.S. synthetic polymer industry which contributes strongly to national productivity. The program develops concepts, measurements, standards, and data that can be used to insure the reliable performance and effective use of polymers in solving national problems including the growth of industrial productivity, improved national security, more efficient government, a more scientific basis for regulation, improved health, and better materials utilization.

*600,638*
**PB87-132262** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Chain Configurations in Lamellar Semicrystalline Polymer Interphases.**
Final rept.,
J. A. Marqusee, and K. A. Dill. 1986, 7p
Pub. in Macromolecules 19, n9 p2420-2426 1986.

Keywords: *Polymers, Lamellar structure, Reprints, Interphases.

A mean-field lattice theory is developed to describe the configurations of long-chain molecules at the crystal/amorphous interface in semicrystalline polymers. Chains are assumed to satisfy continuity and space-filling requirements. The theory permits systematic levels of approximation for correlations among neighboring bonds along the chains subject to the interfacial constraints. The authors consider the two lowest levels of approximation here: (i) single bonds (two segments) or (ii) bond pairs (three segments). Both models predict that approximately 73% of the chains which emerge from the crystal reenter at sites which are immediately adjacent and that the interfacial region should therefore be small, provided the chains are freely flexible. The models predict that the ratio of chain loops to ties in the amorphous region is smaller, and the mean lengths are greater, than predicted by random walk models.

*600,639*
**PB87-134805** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Thermal Crosslinking Procedure for Preparing Solvent-Stable Polymer-Film Electrodes.**
Final rept.,
E. A. Blubaugh, W. C. Bushong, S. I. Shupack, and R. A. Durst. 1986, 9p
Pub. in Analytical Letters 19, n17-18 p1777-1785 1986.

Keywords: *Crosslinking, *Polymeric films, Electrodes, Porphyrins, Reprints.

Published procedures for polymer-film electrodes often give unsatisfactory results because of instability of the film-electrode interface or film dissolution. The authors report a procedure which involves the thermal crosslinking of polymer-film electrodes. These polymer films, prepared from a poly(vinylpyridine/styrene) copolymer, are stable toward a variety of solvents both polar and nonpolar. Electrochemical evaluation of these crosslinked polymer films after chemical derivatization with transition metal-porphyrin complexes is described. The electrochemical studies show that these catalyst-derivatized, polymer-film electrodes are stable for long periods of extended potential cycling through the observed redox couples. Also, the magnitude of the observed currents and peak separation indicates very facile electron transport and small uncompensated film resistance.

*600,640*
**PB87-136693** PC **A06**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Institute for Materials Science and Engineering, Polymers: Technical Activities 1986.**
Annual rept. 1 Oct 85-30 Sep 86,
L. E. Smith, and B. M. Fanconi. Nov 86, 103p
NBSIR-86/3437
See also PB86-196771.

Keywords: *Polymers, Chemical properties, Mechanical properties, Standards, Processing, Composite materials, Durability, Technical activities.

Technical Activities of the Polymers Division for FY 86 are reviewed. Included are descriptions of the 6 Tasks of the Division, project reports, publications, and other technical activities.

*600,641*
**PB87-140208** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Towards a Theory for the Orientation Dependent Packing Entropy of Inhomogeneous Polymer Systems,**
P. van der Schoot. Nov 86, 75p NBSIR-86/3466

Keywords: *Entropy, *Polymers, Orientation, Thermodynamic properties, Liquid crystals.

The report can be thought of as consisting of three parts. In the first part a review is given of Di Marzio's site fraction concept to calculate the configurational entropy of polymers in a homogeneous system. The second part is concerned with Monte Carlo calculations, performed to check the validity of this concept. Results are presented of the packing of rigid, rodlike polymer chains on a square lattice, in the spirit of earlier work by McCrackin. The third and last part of the report deals with the application of the site fraction treatment to the calculation of the configurational entropy of a polymeric system having a density gradient in one direction.

## General

*600,642*
**PB86-197100** PC **A02**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**SRM 1970: Succinonitrile Triple-Point Standard--A Temperature Reference Standard Near 58.08C.**
Final rept.,
B. W. Mangum, and S. El-Sabban. Mar 86, 25p
NBS/SP-260/101
See also PB86-166782. Also available from Supt. of Docs as SN003-003-02722-7. Library of Congress catalog card no. 86-600505. Prepared in cooperation with National Inst. for Standards, Cairo (Egypt).

Keywords: *Succinonitrile, *Temperature measurement, *Standards, Calibrating, *Standard reference materials.

Triple-point-of-succinonitrile cells have been tested and established as Standard Reference Material (SRM) 1970. Of the 115 cells tested, 109 were accepted as SRM 1970. Five of the 115 cells had triple-point temperatures lower than 58.0785 deg.C (the low-temperature limit established for SRM 1970) and, consequently, were rejected. One of the 115 cells broke during tests on it. The mean value of the triple-point temperatures (obtained by freezing) of the 109 cells is 58.0796 plus or minus 0.0015 deg.C, where the uncertainty is the total estimated uncertainty relative to the International Practical Temperature Scale of 1968, Amended Edition of 1975. The standard deviation of the triple-point temperatures is 0.48 mK. The purity of the succinonitrile of the SRM 1970 cells is estimated to range from 99.999,97% to 99.999,84%. The preparation of the cells, the various tests performed on them,

and the procedure recommended for their use are described.

*600,643*
**PB86-227592** PC **A08**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**NBS (National Bureau of Standards) Standard Reference Materials Catalog 1986-87,**
Special pub.,
R. W. Seward. Jun 86, 165p NBS/SP-260
Supersedes PB84-165349. Also available from Supt. of Docs as SN003-003-02740-5.

Keywords: *Catalogs(Publications), Standards, *Standard reference materials.

The catalog describes the Standard Reference Materials (SRM's) currently available from the National Bureau of Standards (NBS), lists those in preparation, and provides ordering information. The descriptions provide nominal values for these SRM's. Certified values are provided in the certificates that accompany each SRM. Price Lists for SRM's are issued as separate supplements to the catalog and include new SRM's as they are issued.

*600,644*
**PB87-100186** PC **A08**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Journal of Research of the National Bureau of Standards, Volume 91, Number 3, May-June 1986.**
Jun 86, 166p
See also PB87-100194 through PB87-100244 and PB86-206364. Also available from Supt. of Docs as SN703-027-00010-5.

Keywords: *Research, Chemical analysis, Heat measurement, Chemical reactions, Thermal analysis, Enthalpy, Electric switches, Temperature control, Carbinols, Metalloids, Pipe flow, Unsteady flow, Calorimetry, Differential scanning calorimetry, Biotechnology.

Table of contents includes: High precision microcalorimetry: Apparatus, procedures, and biochemical applications; Standards development for differential scanning calorimetry; Miniature mercury contact switches for instrument temperature control; Thermophysical property measurement on chemically reacting systems--a case study; Inorganic materials biotechnology: A new industrial measurement challenge; Improvements in the application of the numerical method of characteristics to predict attenuation in unsteady partially filled pipe flow.

*600,645*
**PB87-100210**
(Order as PB87-100186, PC **A08**/MF **A01**)
National Bureau of Standards (NEL), Boulder, CO.
**Miniature Mercury Contact Switches for Instrument Temperature Control,**
T. J. Bruno, and J. G. Shepherd. Jun 86, 3p
Sponsored by Gas Research Inst., Chicago, IL., and Department of Energy, Washington, DC.
Included in Jnl. of Research of the National Bureau of Standards, v91 n3 p131-133 May-Jun 86.

Keywords: *Electric switches, *Mercury, Temperature control, Temperature measuring instrument.

In this short note the authors described the design and construction of several modifications of miniature mercury contact switches for use in laboratory temperature control applications. Commerical contact switches, or contact thermometers as they are commonly called, are limited in their application because of their large size. The units which we present here are much more compact and are thus suitable for a wider range of applications. The limitations of the miniature contact switches in their present configurations are also discussed.

*600,646*
**PB87-128179** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Comment on 'Convection Currents In a Water Calorimeter'.**
Final rept.,
S. R. Domen. 1986, 3p
Pub. in Physics in Medicine and Biology 31, n10 p1166-1168 1986.

Keywords: *Calorimeters, *Convection, Ionizing radiation, Water, Thermistor, Reprints.

Schulz and Weinhous (Phys. Med. Biol., 1985 30, 1093-1099) detected convection currents in a water calorimeter irradiated with broad horizontal beams of 25-MV x rays and 19-MeV electrons. The region of particular interest is near the beam entrance wall. Considering their recorded results, the broad beams and large electrical powers dissipated in the sensing thermistors, and calculations which approximately describe the convective velocity stream, it is hypothesized that most of the observed convective effects could have been caused by convective cooling of the sensors.

*600,647*
**PB87-137154** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Journal of Research of the National Bureau of Standards, Volume 91, Number 6, November-December 1986.**
Dec 86, 56p
See also PB87-137162 through PB87-137188, and PB87-121315. Also available from Supt. of Docs as SN703-027-00013-0.

Keywords: *Research, Chemical analysis, Gases, Gallium, Atomic mass, Thermal expansion, Platinum, Temperature dependence, Isotope ratio, Reference materials, Platinum rhodium alloys.

The report includes the folliwng papers: The temperature dependence of spectral broadening in the Hg (6 singlet S(sub 0) - 6 triplet P(sub 1)) Multiplet at high optical densities; Absolute isotopic abundance ratio and atomic weight of a reference sample of gallium; Thermal expansion of platinum and platinum-rhodium alloys.

# CIVIL ENGINEERING

## Civil Engineering

*600,648*
**PB86-192473** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Thermal Resistivity of Soils.**
Final rept.,
L. A. Salomone, and W. D. Kovacs. 1984, 15p
Pub. in Jnl. of the Geotechnical Engineering Division, American Society of Civil Engineers 110, n3 p375-389 1984.

Keywords: *Thermal conductivity, *Soils, *Civil engineering, Plasticity, Cost analysis, Atterberg limits, Moisture contents, Heat transfer, Soil tests, Reprints.

Information on the thermal properties of soils from different disciplines of science and engineering is consolidated for the purpose of identifying low cost, simple procedures for assessing the variation of the thermal resistivity of soils with changes in moisture content. Three procedures for determination of the critical moisture content are presented. The critical moisture content is the moisture content at the knee of the thermal resistivity versus moisture content curve.

*600,649*
**PB86-193893** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Thermal Performance of Fine-Grained Soils.**
Final rept.,
L. A. Salomone, W. D. Kovacs, and T. Kusuda. 1984, 16p
Pub. in Jnl. of the Geotechnical Engineering Division, American Society of Civil Engineers 110, n3 p359-374 1984.

Keywords: *Soil compacting, *Civil engineering, Thermal conductivity, Atterberg limits, Bearing capacity, Moisture content, Optimization, Plasticity, Reprints, AASHTO standards.

Laboratory thermal probe tests performed on an AASHTO standard reference material (a silty clay) showed that thermal resistivity (C cm/watt) varies with soil moisture content and dry density. The tests were performed to correlate soil thermal behavior with the limit states of fine-grained soils. Over 80 thermal resistivity measurements were made on specimens compacted to various densities and moisture contents. Results are presented which indicate that the optimum moisture content and the plastic limit can be correlated with the thermal behavior of fine-grained soils.

*600,650*
**PB86-230976** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Reflections on the Presentations: Technology and the Future of the U.S. Construction Industry.**
Final rept.,
J. G. Gross. 1986, 4p
Pub. in Proceedings of the Panel on Technical Change and the U.S. Building Construction Industry, Washington, DC., August 29-30, 1984, p150-153 1986.

Keywords: *Buildings, *Construction industry, Productivity, Technology assessment.

Provides comments and observations for the OTA Panel on Technology Changes and Impacts on the Building Construction Industries. It addresses needs for improving the application of computers to construction and particularly the need for interface standards. Arguments are made for advances in education of construction professionals and the opportunity for research to improve productivity. Other research needs discussed are indoor air quality and diagnostics.

## Construction Equipment, Materials, & Supplies

*600,651*
**PB86-160090** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Cement in the 1990s: Challenges and Opportunities.**
Final rept.,
G. Frohnsdorff, and J. Skalny. 1983, 14p
Pub. in Philosophical Transactions of the Royal Society of London, Series A 310: Mathematical and Physical Sciences, p17-30 1983.

Keywords: *Cements, Utilization, Performance standards, Forecasting, Standards, Reprints.

Despite large gaps in knowledge of cement science, cement and concrete are the preferred materials for much civil engineering construction. As the gaps are filled, cement and concrete should become even more valuable construction materials. The gaps stem in large part from the inability to characterize cements and their hydration products in unambiguous terms. For many reasons, there have been significant barriers to cement research. The barriers have resulted in fragmentation of research efforts among groups with less than adequate mixtures of skills. Nevertheless, the authors believe there will be a revolution in cement technology based on an integration of research efforts through cooperation on national and international levels.

*600,652*
**PB86-192135** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Shear Resistance of Unreinforced Hollow Concrete Block Masonry Walls.**
Final rept.,
K. Woodward, and F. Rankin. 1985, 15p
Pub. in Proceedings of North American Masonry Conference (3rd), Arlington, TX., June 3-5, 1985, p38-1 - 38-15.

Keywords: *Concrete blocks, Masonry, Shear strength.

An experimental investigation is described which has as its primary focus the determination of shear resistance exhibited by unreinforced, ungrouted, hollow concrete block masonry walls. Thirty-two wall panel tests are reported. The parameters in the investigation include the amount of applied vertical compressive stress, wall aspect-ratio, block strength and mortar type.

*600,653*
**PB86-193125** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Fluorescent Thin Sections to Observe the Fracture Zone in Mortar.**
Final rept.,
L. I. Knab, H. N. Walker, J. R. Clifton, and E. R. Fuller. 1984, 6p
Pub. in Cement and Concrete Research 14, n3 p339-344 May 84.

Keywords: *Mortars(Materials), *Fracturing, Fluorescence, Fracture properties, Cracking(Fracturing), Concretes, Microstructure, Reprints.

The report deals with the use of fluorescent thin sections to observe the microstructural details of the fracture zone. A mortar is used to illustrate the technique. It is concluded that the fluorescent thin section technique has the potential of providing a valuable new source of information on the microstructural details of the fracture zone in mortars and concretes, both near the surface and in the interior of specimens.

*600,654*
**PB86-196425** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Calcium Hydroxide Distribution and Calcium Silicate Hydrate Composition in Tricalcium Silicate and Beta-Dicalcium Silicate Pastes.**
Final rept.,
H. F. W. Taylor, and D. E. Newbury. 1984, 6p
Pub. in Cement and Concrete Research 14, n1 p93-98 Jan 84.

Keywords: *Silicate cements, Calcium hydroxides, Calcium silicates, Microanalysis, Reprints.

Pastes of C3S and B-C2S 23 years old were studied by electron probe microanalysis. In both cases, regions consisting entirely or largely of calcium hydroxide and of C-S-H were distinguished on a scale of 2-50 um. The regions high in C-S-H accounted for 75-80 percent of the whole in the C3S paste and about 96 percent in the C2S paste; these values are much higher than those initially occupied by anhydrous starting materials. Within the high C-S-H areas, no variation was detected that could have corresponded to the so-called inner and outer hydrates. The ratio of mean Ca to mean Si in the high C-S-H areas was 1.72 for the C3S and 1.78 for the C2S paste, but because of possible admixture with calcium hydroxide on or below a micrometer scale, the Ca/Si ratio of the C-S-H may be as low as 1.5.

*600,655*
**PB86-196433** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Electron Microprobe Study of a Mature Cement Paste.**
Final rept.,
H. F. W. Taylor, and D. E. Newbury. 1984, 9p
Pub. in Cement and Concrete Research 14, n4 p565-573 Jul 84.

Keywords: *Portland cement, Electron microscopy, Electron probes, X ray analysis, Silicate cements, Reprints.

A portland cement paste 23 years old, and essentially fully hydrated, was studied by electron probe microanalysis. X-ray images indicated that the distributions in space of the original, largely polymineralic cement grains, and of the individual phases within them, are substantially preserved in the hydrated material. This was shown especially clearly by the Mg and Fe images, probably because these elements do not readily migrate in the alkaline medium.

*600,656*
**PB86-213378** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Investigation of the Corrosion of Aluminum Standing-Seam Roofing at an Army Facility,**
R. G. Mathey. Jun 86, 21p NBSIR-86/3387
Sponsored by Construction Engineering Research Lab. (Army), Champaign, IL., and Defense Logistics Agency, Alexandria, VA.

Keywords: *Roofing, *Aluminum, Corrosion, Weathering.

An investigation was conducted to determine the extent of corrosion of an aluminum standing-seam roofing system exposed to weathering over a period of nearly three years. The aluminum roofing was installed on three large warehouses at an Army facility in Columbus, Ohio. A high performance elastomeric sealant was used in forming the standing seams of the roofing system. The roof slope, about 5 percent, was less than that usually recommended for unsoldered standing-seam roofing. The roofs were located in a region having a high level of acid rain.

*600,657*
**PB86-238268** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Calcium Aluminate Cements.**
Final rept.,
G. J. Frohnsdorff, and J. E. Kopanda. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v1 p472-474 1986.

Keywords: *Aluminate cements, Cements, Calcium, Reprints.

No abstract available.

*600,658*
**PB86-238276** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Portland Cements, Blended Cements and Mortars.**
Final rept.,
G. J. Frohnsdorff. 1986, 8p
Pub. in Encyclopedia of Materials Science and Engineering, v5 p3847-3854 1986.

Keywords: *Cements, Portland cements, Mortars(Material), Reprints.

No abstract available.

*600,659*
**PB86-238284** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Cements, Specialty.**
Final rept.,
G. Frohnsdorff. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v1 p575-579 1986.

Keywords: *Cements, Reprints.

No abstract available.

*600,660*
**PB86-238292** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Building Materials: Nondestructive Evaluation.**
Final rept.,
J. R. Clifton. 1986, 4p
Pub. in Encyclopedia of Materials Science and Engineering, v1 p446-449 1986.

Keywords: *Construction materials, Nondestructive tests, Reprints.

No abstract available.

*600,661*
**PB87-106753** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Point Source-Point Receiver, Pulse-Echo Technique for Flaw Detection in Concrete.**
Final rept.,
N. J. Carino, M. Sansalone, and N. N. Hsu. 1986, 10p
Pub. in Jnl. of the American Concrete Institute 83, n2 p199-208 1986.

Keywords: *Concretes, *Nondestructive tests, Greens function, Wave propagation, Impact, Reprints.

Numerical and experimental results are presented on the use of a point source point receiver, pulse-echo technique to locate flaws within hardened concrete. A large concrete slab was cast with known internal flaws which were created by embedded polyurethane foam disks, ranging from 5 to 50 cm in diameter. Using steel balls dropped onto the slab surface as a point source and a conical, broadband, displacement transducer with a small contact area as a point receiver, the ability of the technique to locate the embedded disks was evaluated. Numerical solutions for the response of an infinite plate to surface impact were used to help interpret experimental signal traces. Boundaries of both planar and inclined disks were determined to within a few centimeters. Thus, it was concluded that the proposed technique can be a reliable nondestructive test method for detecting flaws and discontinuities within hardened concrete. The inherent limitations of the method are alse discussed.

## Highway Engineering

*600,662*
**PB87-145413** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Measuring the Corrosion Rate of Reinforcing Steel Concrete - Final Report,**
E. Escalante, E. Whitenton, and F. Qiu. Oct 86, 50p NBSIR-86/3456
See also report dated Apr 84, PB84-144532. Sponsored by Federal Highway Administration, Washington, DC.

Keywords: *Reinforcing steels, *Corrosion tests, *Bridge decks, Highway bridges, Reinforced concrete, Bars, Nondestructive tests, Computer programs, Frederick County(Maryland).

The report describes a two phase study directed at developing a portable system for measuring the corrosion of steel in concrete bridge decks. A small, portable computer system is used to control the measurement of polarization resistance of steel in concrete, and using current interruption, iR compensation is accomplished. During the development stage, measurements were made on small specimens in a laboratory controlled environment, and the results of the calculated weight loss measurements based on the electrochemical measurement are compared to gravimentrically determined weight loss. In the second phase, the portable system was used to measure the corrosion of three bridge decks in Frederick County, Maryland, over a four month period. The results of these field measurements and the problems encountered are discussed.

## Soil & Rock Mechanics

*600,663*
**PB87-103297** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Study of Reverse Torque Ratio in the Helical Probe Test,**
F. Y. Yokel, and K. Y. Chung. Sep 86, 27p NBSIR-86/3423
Prepared in cooperation with Korea Inst. of Science and Technology, Seoul.

Keywords: *Soil properties, *Augers, *Grain size, Helical gears, Torque, Field tests, Data, Soil tests.

The report covers a study to determine whether the ratio of the torque required to extract the Helical Test Probe to the torque required to advance the probe (the reverse torque ratio) can be used to determine the average grain size of the soil. On the basis of 274 test points in sandy, silty, and clayey soils, it was concluded that the reverse torque ratio decreases with increasing average grain size. The relation between grain size and reverse torque ratio is apparently not sensitive to the magnitude of the torque required to advance the probe.

# COMBUSTION, ENGINES, & PROPELLANTS

## Combustion & Ignition

*600,664*
**PB86-171089** PC **A04**/MF **A01**
Case Western Reserve Univ., Cleveland, OH. Dept. of Mechanical and Aerospace Engineering.
**Rate Constants for Polymethyletacrylate Diffusion Flame Using a Semi-Global Reaction Model.**
Final rept.,
N. A. Messaoudene, and J. S. Tien. Feb 86, 59p NBS/GCR-86/508
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Combustion, *Diffusion flames, Polymethyl methacrylate, Reaction kinetics, Extinction.

A numerical study of the combustion and extinction in the stagnaion point boundary layer of a condunsed fuel (PMMA) has been performed using a three-step semi-global reactions model. In the first step considered, fuel is oxidized to form carbon monoxide and water vapor. In the second, carbon monoxide is oxidized to form carbon dioxide, and in the third reaction, carbon dioxide decomposes into carbon monoixde and oxygen, which is the reverse of the second reaction. The governing equations were transformed into a set of ordinary differential equations through a similarity variable. Fictitions unsteady terms were added to the ordinary differential equations and the resulting equations were solved numerically using an explicit scheme for the fictitions unsteady terms. Use has been made of Howard, et. al., kinetics constants for the forward reaction of CO (second reaction), and constants calculated from equilibrium considerations for the backward reaction (third reaction). Comparing the extinction results with experimental data, good agreement was found for B sub F = 4.43 x 10 to the 13th power cu ml/gmole.sec. and E sub F = 32000 cal/mole, which are respectively the preexponential factor and the activation energy for the rate of the first reaction.

*600,665*
**PB86-171170** PC **A08**/MF **A01**
Case Western Reserve Univ., Cleveland, OH. Dept. of Mechanical and Aerospace Engineering.
**Diffusion Flame Stabilization at the Leading Edge of a Fuel Plate.**
Final rept.,
C. H. Chen, and J. S. Tien. Feb 86, 173p NBS/GCR-86/509
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Combustion, *Diffusion flames, Computer programs, Stability, Computerized simulation.

A theoretical model of a laminar diffusion flame at the leading edge of a fuel plate in a forced convective flow is presented and solved numerically to study the flame stabilization and blowoff phenomena. The system of governing equations consists of the two-dimensional Navier-Stokes' momentum, energy and species equations with a one-step overall chemical reaction and second-order, finite rate Arrhenius kinetics. The computation is performed over a wide range of Damkohler numbers. For large Damkohler numbers, envelope flames are found to exist where the computed fuel evaporation rate, the flame stand-off distance and the velocity profiles show certain similitude. As Damkohler number is lowered, a transition to open-tip flame takes place where the flame becomes stabilized on the sides of the fuel plate. Further decreasing of the Damkohler number pushes the diffusion flame downstream out of the leading edge region. In the paper, the flame structures of the envelope and the open-tip flames are presented together with a description of the transition sequence. The implication of the work to downstream boundary layer combustion is also discussed.

*600,666*
**PB86-182813** PC **A03**/MF **A01**
Case Western Reserve Univ., Cleveland, OH. Dept. of Mechanical and Aerospace Engineering.
**Effect of Convective Velocity on Upward and Downward Burning Limits of PMMA (Polymethylmethacrylate) Rods.**
Final rept.,
Y. Halli, and J. S. T'ien. Feb 86, 42p NBS/GCR-86/507
Grant NANB-D0013
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Burning rate, *Combustion physics, *Polymethyl methacrylate, Oxygen, Velocity, Flames.

Limiting oxygen mole fractions for 1.27 centimeter PMMA rods in upward and downward self-sustained burnings are measured as a function of the oxygen/nitrogen mixture flow velocity. For downward burning, the limiting oxygen mole fractions are found to be essentially independent on the flow velocity in the range between 5 to 40 cm/sec and increases when velocity is greater than 40 cm/sec. In the upward burning configuration, a stronger and non-monotonic velocity dependence is discovered. The limiting oxygen percentage reaches a minimum at a velocity of 12 cm/sec and increases in both directions as the mixture velocity increases or decreases. The minimum limiting oxygen mole fractions are, for the downward case, 0.184 and for the upward case, 0.15. Upward flame propagation limits in the presence of a small pilot flame have also been determined for PMMA rod. It is demonstrated that flames can propagate in an environment with an oxygen mole fraction lower than its critical extinction value for self-sustained flames.

*600,667*
**PB86-183548** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Smoldering Combustion,**
T. J. Ohlemiller. Feb 86, 33p NBSIR-85/3294

Keywords: *Combustion, Cellulose, Toxicity, Fire safety, Fire hazards, *Smoldering.

Smoldering combustion is a common fire safety hazard that contributes substantially to the fire losses in the United States; fire protection engineers thus have a need to be familiar with its characteristics. The post-initiation behavior of smoldering (self-sustaining propagation and transition to flaming) is described here. The most studied cases of propagation are one-dimensional; the underlying mechanisms are described qualitatively and spread rates for several materials are presented along with limited information on toxic gas evolution.

*600,668*
**PB86-189677** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Validation of Network Models for Smoke Control Analysis.**
Final rept.,
J. H. Klote, and X. Bodart. 1985, 7p
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 91, n2 pt2 p1134-1145 1985.

Keywords: *Smoke, Buildings, Air flow, Simulation, Reprints, *Smoke control.

Currently there are many buildings with systems intended to control smoke movement in building fire situations. Network computer models have been developed to analyze these systems for research and design purposes. The paper presents a general description of such models, a discussion of validation techniques used to check the computer algorithms, and the results of full scale tests conducted in a pressurized stairwell at Champs Sur Marne, France to validate the basic assumptions of these computer models.

*600,669*
**PB86-189883** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Nylons: A Review of the Literature on Products of Combustion and Toxicity,**
E. Braun, and B. C. Levin. Feb 86, 89p NBSIR-85/3280
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Polyamide resins, *Nylon 6, *Combustion products, *Toxicity, Pyrolysis, Reviews, Laboratory animals.

The English literature through 1984 on polyamides was reviewed to determine the nature of the combustion products and their toxicity. The review was limited to aliphatic polyamides normally called nylon and excludes aromatic polyamides such as Nomex and bicomponent polymers. Typical pyrolysis products from a broad range of nylons do not appear to differ greatly. Many of the decomposition products detected in vacuum pyrolysis experiments appear as products of thermal degradation in inert and air atmospheres. In air, a general reduction in the quantities of heavier hydrocarbons is noted along with an increase in the production of CO, CO2, H2O, NH3, HCN, and NOx. The toxicity of the thermal degradation products from various types of nylon has been evaluated by nine different protocols. Reported LC50 values range from 10.8 mg/l to 61.9 mg/l. Dyes apparently do not affect the materials' combustion products toxicity, but an increase in the amount of backcoating on a nylon fabric increase toxicity. Time to death measurements show that volatile products from nylons are less toxic than those from rayons or cotton, while the blending of wool with nylon greatly increase the toxicity of the thermal decomposition products. In general, however, the overall toxicity of the thermal degradation products from nylon do not appear to be greatly different than those from many other polymeric materials.

*600,670*
**PB86-195815** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Modeling of Smoldering Combustion Propagation.**
Final rept.,
T. J. Ohlemiller. 1985, 34p
See also PB84-236389.
Pub. in Progress in Energy and Combustion Science 11, p277-310 1985.

Keywords: *Combustion, *Cellulosic resins, Fire hazards, Reprints, *Smoldering, Polyurethanes.

Smoldering combustion of various natural and synthetic solid materials constitutes a substantial fire hazard; the process itself produces copious toxic gases and it can lead to flaming combustion. The review focuses on the coupled chemical and physical processes invovled in self-sustained propagation of smoldering. The potential heat sources (gas-phase oxidation, oxidative polymer degradation char oxidation) are examined along with the heat sinks (polymer pyrolysis, water vaporization). It is concluded that even for the most-studied case of cellulose, the chemical mechanisms involved in these processes are both too complex and too poorly understood to be included in a smolder propagation model.

*600,671*
**PB86-202074** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Overview of Dioxin Formation in Gas and Solid Phases Under Municipal Incinerator Conditions.**
Final rept.,
W. M. Shaub, and W. Tsang. 1983, 2p
Sponsored by American Chemical Society, Washington, DC.
Pub. in Proceedings of the National Meeting, American Chemical Society, Division of Environmental Chemistry (186th), Washington, DC, August 28-September 2, 1983, v23 n2 p267-268.

Keywords: *Incinerators, Combustion, Fly ash, Gases, Oxygen heterocyclic compounds, Chlorine organic compounds, *Dioxin(Herbicides), Solid wastes, Dibenzodioxin/tetrachloro.

Mechanisms for the formation of dioxins during incineration via gas and gas-fly ash interactions are presented and discussed. On the basis of simplifying assumptions analytical expressions which relate dioxin formation with elementary reactions are derived. A previous conclusion regarding the inability of the former to account for reported emissions from municipal incinerators is reinforced. For the latter, experimental observations are used to derive relevant rate parameters. While these do not appear to be unreasonable, direct experimental verification is required.

*600,672*
**PB86-204617** PC **A06**/MF **A01**
Pennsylvania State Univ., University Park. Dept. of Mechanical Engineering.
**Structure of Adiabatic Wall Plumes,**
M. C. Lai, and G. M. Faeth. Nov 85, 106p NBS/GCR-86/503
Grant NANB-4D0032
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Plumes, Turbulence, Buoyancy, Velocity measurement, Walls, Cross correlation.

A theoretical and experimental study of turbulent buoyancy plumes along plane surfaces is described. These flows are of interest since their hydrodynamic properties are similar to wall fires and they can be studied without complications due to combustion and radiation. Wall plumes were generated by carbon dioxide/air mixtures flowing from a slot at the top of the wall (since the flows were negatively buoyant). The following measurements were made; mean and fluctuating velocities and Reynolds stresses, using laser Doppler anemometry (LDA); mean and fluctuating concentrations, using laser-induced fluorescence (LIF); and velocity/concentration correlations, using combined LDA/LIF. The flows were also analyzed using a mixing-length model and a k-epsilon-g turbulence model (both ignoring buoyancy/turbulence interactions). Buoyancy/turbulence interactions were significant in the present flows; therefore while predictions of mean properties were reasonably good, turbulence quantities were underestimated.

*600,673*
**PB86-215159** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Buoyancy Driven Flow as the Forcing Function of Smoke Transport Models.**
Final rept.,
W. W. Jones, and X. Bodart. May 86, 27p NBSIR-86/3329

Keywords: *Smoke, Flow distribution, Buoyancy, Numerical analysis, *Fire models.

Flow at vents is the major driving force in smoke transport models. The precision with which we can calculate these flows determines to a great extent how accurately we can model buoyant flow and the inherent speed of the models. This report describes some of the problems encountered in calculating these flows, and gives a general algorithm for their calculation.

*600,674*
**PB86-230943** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Buoyant Source In the Lower of Two, Homogeneous, Stably Stratified Layers.**
Final rept.,
L. Y. Cooper. 1984, 7p
Sponsored by Department of Health and Human Services, Washington, DC., Federal Aviation Administration, Washington, DC., and Department of the Interior, Washington, DC.
Pub. in Proceedings of International Symposium on Combustion (20th), Ann Arbor, MI., p1567-1573 1984.

Keywords: *Buoyancy, *Plumes, *Fires, Layers, Heat transfer, Turbulent flow.

A point source of buoyancy is located at a specified elevation within the lower of two, homogeneous, stably stratified layers. A turbulent buoyant plume is formed above the source, and it impinges on the layers' interface. Derives and solves a set of model equations for these plume-interface interactions, and the results are applied to a generic heat transfer problem related to fires in enclosures.

*600,675*
**PB86-232410** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Development of an Automated Probe Positioner for Measurements in Fire-Generated Plumes and Ceiling Jets,**
D. W. Stroup. May 86, 46p NBSIR-86/3379

Keywords: *Probes, *Plumes, Temperature measurement, Gas burners, Measurement, Velocity, *Ceiling jets.

The report describes the development of an automated probe positioner. The system has been used for extensive measurements of temperatures at a large number of positions within a laboratory-scale fire-flow experimental apparatus. In its present configuration, the device is designed to operate within a 1.22 m diameter cylindrical enclosure. The apparatus has horizontal, vertical, and rotational motion capabilities. A single microcomputer is used to control probe positioning, perform data-taking, and evaluate statistical results. These statistical results are used by the system to determine the number of data points to record at a given position.

*600,676*
**PB87-110029** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Chemical Kinetic Data Base for Combustion Chemistry. Part 1. Methane and Related Compounds,**
W. Tsang, and R. F. Hampson. c1986, 190p
Included in Jnl. of Physical and Chemical Reference Data, v15 n3 p1087-1289 1986. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Methane, *Combustion, Chemical reactions, Thermodynamic properties, Oxidation, Pyrolysis, Transport properties, Aromatic hydrocarbons, Aliphatic hydrocarbons, Chemical reaction kinetics.

The document contains evaluated data on the kinetics and thermodynamic properties of species that are of importance in methane pyrolysis and combustion. Specifically, the substances considered include H, H2, O, O2, OH, HO2, H2O2, H2O, CH4, C2H6, HCHO, CO2, CO, HCO, CH3, C2H5, C2H4, C2H3, C2H, CH3CO, CH3O2, CH3O, singlet CH2, and triplet CH2. All possible reactions are considered. In arriving at recommended values, first preference is given to experimental measurements. Where data do not exist, a best possible estimate is given. In making extrapolations, extensive use is made of RRKM calculations for the pressure dependence of unimolecular processes and the BEBO method for hydrogen transfer reactions. In the total absence of data, recourse is made to the principle of detailed balancing, thermokinetic estimates, or comparisons with analogous reactions. The temperature range covered is 300-2500 K and the density range 1 x 10 raised to the 16th power - 1 x 10 raised to the 21st power molecules/cc. This data base forms a subset of the chemical kinetic data base for all combustion chemistry processes.

*600,677*
**PB87-121349**
(Order as PB87-121315, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Multi-kilogram Capacity Calorimeter for Heterogeneous Materials,**
K. L. Churney, A. E. Ledford, M. L. Reilly, and E. S. Domalski. 24 Apr 86, 22p
Included in Jnl. of Research of the National Bureau of Standards, v91 n5 p277-298 Sep-Oct 86.

Keywords: *Enthalpy, *Combustion, *Calorimeters, Thermodynamic properties, *Solid wastes.

A large capacity calorimeter was designed and constructed in order to determine the enthalpies of combustion of kilogram-size samples of municipal solid waste (MSW) in flowing oxygen near atmospheric pressure. The combustion of the organic fraction of the samples was complete to greater than 99.9+%. The percent coefficient of variation (100 X standard deviation/average), % CV, of calibration measurements using microcrystalline cellulose was 0.2%. The % CV of the measurements of the enthalpy of combustion of a processed MSW sample was 0.4%. The combined systematic errors due to departure from usual design standards and conventional operating procedures is estimated to be less than 0.4% of the calorific value.

*600,678*
**PB87-122800** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Ignition and Combustion Temperatures Determined by Laser Heating.**
Final rept.,
J. W. Bransford. 1985, 20p
Contract NASA-H-43201(B)
Sponsored by National Aeronautics and Space Administration, Huntsville, AL. George C. Marshall Space Flight Center.
Pub. in Flammability and Sensitivity of Materials in Oxygen-Enriched Atmospheres: Second Volume, ASTM STP 910, p78-97 1985.

Keywords: *Ignition, *Combustion, Aluminum alloys, Nickel alloys, Stainless steels, Reprints, Laser-radiation heating, Steel S30200, Nickel alloy N07718, Nickel alloy N04400, Aluminum alloy A96061.

A laser heating technique and facility have been developed to study metal ignition and combustion in high-pressure oxygen. The ignition and combustion temperatures, estimates of oxidation rates, and ignition and combustion morphology can be determined. This facility and the laser heating techniques are described. Examples of the type of data obtained are presented and discussed. The ignition temperature curves for an aluminum alloy-Unified Numbering System (UNS) A96061, a stainless steel-UNS S30200, and two nickel alloys-UNS N07718 and N04400 are given.

*600,679*
**PB87-123196** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Ignitability Measurements with the Cone Calorimeter,**
V. Babrauskas, and W. J. Parker. Sep 86, 50p NBSIR-86/3445

Keywords: *Calorimeters, *Ignition, Heat measurement, Combustion, Flammability, Plastics, Particle boards.

The Cone Calorimeter is a new-generation instrument developed primarily for making rate of heat release measurements. The instrument, containing a uniform and well-characterized irradiance source, was also seen to be useful for making measurements of radiant ignition on materials. Data have now been collected for a wide range of materials. The effects of various apparatus dependencies are discussed. Also, some comparative data are available illustrating the performance of similar materials in other apparatuses. Finally, for a selected material, Douglas fir particle board, a detailed comparison with an ignition model has been made.

*600,680*
**PB87-128005** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Upward Turbulent Flame Spread.**
Final rept.,
K. Saito, J. Quintiere, and F. A. Williams. 1986, 12p
Pub. in Proceedings of International Symposium on Fire Safety Science (1st), Gaithersburg, MD., October 7-11, 1985, p75-86 1986.

Keywords: *Flames, *Combustion, Polymethyl methacrylate, Wood particle boards, Fire tests, Time dependence.

Mechanisms and rates of upward spread of turbulent flames along thermally thick vertical sheets are considered for both noncharring and charring fuels. By addressing the time dependence of the rate of mass loss of the burning face of a charring fuel, a linear integral equation of the Volterra type is derived for the spread rate. Measurements of spread rates, of flame heights and of surface temperature histories are reported for polymethylmethacrylate and for Douglas-fir particle board for flames initiated and supported by a line-source gas burner, with various rates of heat release, located at the base of the fuel face. Sustained spread occurs for the synthetic polymer and not for the wood. Comparisons of measurements with theory aid in estimating characteristic parameters for the fuels.

*600,681*
**PB87-131496** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Optical Tomography in Combustion.**
Final rept.,
R. Goulard, and S. R. Ray. 1985, 21p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Advances in Remote Sensing Retrieval Methods, p71-91 1985.

Keywords: *Combustion, Absorption, Chemical analysis, Tomagraphy, Diagnostic techniques.

The principles of tomography, or multiangular measurements, have only recently been implemented using

visible light. Tomographic absorption measurements, in particular, have a number of advantages over optical point measurement techniques. In addition to the evident potential for rapid two or three dimensional imaging with high temporal and spatial resolution, the technique is also attractive in terms of the signal to noise ratio, due to multiple measurements of any single space element. A brief treatment shows the influence of redundancy, background and Poisson statistics on the overall signal to noise ratio as compared to point scattering techniques. Experimental work on the development of a high speed optical tomography system is presented, demonstrating the capability to measure the two dimensional distribution of temperature and OH concentration in a premixed methane flame within five milliseconds.

*600,682*
**PB87-140190** PC **A04**/MF **A01**
California Univ., Berkeley. Dept. of Mechanical Engineering.
**Fire Propagation in Concurrent Flows.**
Final rept. 1 Aug 85-31 Jul 86,
A. C. Fernandez-Pello. Nov 86, 66p NBS/GCR-86/518
Contract NB83-NADA-4020
See also PB86-181849. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Flame propagation, *Fire tests, Combustion, Numerical analysis, Gas flow, Ignition, Diffusion flames, *Flame spread.

A research program is being carried out to study the mechanisms controlling the spread of fire in a concurrent gas flow. Research performed includes a numerical analysis of the flow assisted spread of flames over the surface of a thermally thick fuel, an experimental study of the extinction and stabilization of a diffusion flame over a flat combustible surface, and a theoretical study of the forced ignition of a vaporizing combustible surface. The flow assisted flame spread analysis incorporates finite rate kinetics in the formulation of the problem. This provides a more accurate description of the regions with slow chemistry such as the upstream leading edge of the flame and the flame tip. The flame extinction experiments compliment a previously developed numerical analysis of the problem. The study addresses the process controlling the structure and stabilization of the upstream leading edge of the flame. The ignition study has as final objective the description of the ignition by a hot particle (firebrand), or by gas absorption of radiation, of a vaporizing surface in a convective flow. During this period, a one-dimensional model of ignition has been developed.

*600,683*
**PB87-140240** PC **A04**/MF **A01**
Factory Mutual Research Corp., Norwood, MA.
**Prediction of Fire Properties of Materials. Part 1. Aliphatic and Aromatic Hydrocarbons and Related Polymers.**
Technical rept.,
A. Tewarson. Dec 86, 61p NBS/GCR-86/521
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Combustion, Aliphatic hydrocarbons, Aromatic hydrocarbons, Combustion products, Polymers, Flammability testing.

Combustion behavior of 82 aliphatic and aromatic hydrocarbons and related polymers has been examined for application to fire models. Quantitative predictions have been made for the following fire properties; combustion efficiency and its convective and radiative components; fraction of unconsumed hydrocarbon and polymer vapors present as hydrocarbons; and generation efficiencies of CO2, CO, particulates and mixture of unidentified carbon compounds.

*600,684*
**PB87-140257** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Time-Dependent Simulation of Small-Scale Turbulent Mixing and Reaction.**
Annual rept. Nov 84-Nov 85,
H. R. Baum, R. G. Rehm, D. M. Corley, and D. W. Lozier. Feb 86, 43p NBSIR-86/3334
Contract AFOSR-ISSA-85-0026
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Combustion, Mathematical models, Chemical reactions, Diffusion, Convection.

A mathematical model of the local transient diffusion-controlled reaction between initially unmixed species is presented. It is intended ultimately as a computational 'molecule' to be imbedded in direct simulations of larger scale reacting flows. The model consists of an interacting three-dimensional strain vortex field which exactly satisfies the Navier-Stokes equation, an analytically determined Lagrangian representation of the mixing process and convection-diffusion equations for the reacting species in Lagrangian coordinates. The length scale established by the stretching of the vorticity field is shown to be directly relatable to the Kolmogoroff scale if the local strain rate has a scale consistent with laminar boundary layer mixing. An analytical solution to the convection-diffusion equation governing the diffusion-controlled reaction is derived. The solution is valid for large Schmidt number and describes the evolution of any initially two-dimensional configuration of reactants. A special two-dimensional case of this model, in which vortex strain is excluded and fuel and oxidizer initially occupy adjacent half-spaces, is also analyzed.

## Rocket Engines & Motors

*600,685*
**PB87-134342** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Vortex Shedding Flow Meter Performance at High Flow Velocities,**
J. D. Siegwarth. Oct 86, 97p NBS/TN-1302
Also available from Supt. of Docs as SN003-003-02777-4. Sponsored by National Aeronautics and Space Administration, Huntsville, AL. George C. Marshall Space Flight Center.

Keywords: *Flow meters, Gas flow, Water flow, Liquid oxygen, Air flow, Cryogenics, *Vortex shedding, Space shuttle.

In some of the ducts of the space shuttle main engines (SSME), the maximum liquid oxygen flow velocities approach 10 times those at which liquid flow measurements are normally made. The hydrogen gas flow velocities in other ducts exceed the maximum for gas flow measurement by more than a factor of 3. The results presented here show from water flow tests that vortex shedding flow meters of the appropriate design can measure water flow to velocities in excess of 55 m/s, which is a Reynolds number of about 2 million. Air flow tests have shown that the same meter can measure flow to a Reynolds number of at least 22 million. Vortex shedding meters were installed in two of the SSME ducts and tested with water flow. Narrow spectrum lines were obtained and the meter output frequencies were proportional to flow to + or - 0.5% or better over the test range with no flow conditioning, even though the ducts had multiple bends preceding the meter location. Meters with the shedding elements only partially spanning the pipe and some meters with ring shaped shedding elements were also tested.

# COMMUNICATION

## Common Carrier & Satellite

*600,686*
**PB86-196391** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Law Enforcement Standards Lab.
**Performance of Amplitude Companded Sideband. Interim Report: A Review and Measurement Plan,**
W. L. Kissick, L. T. Jones, and W. J. Hartman. Apr 86, 74p NBS/GCR-86/511
Prepared in cooperation with National Telecommunications and Information Administration, Boulder, CO. Inst. for Telecommunication Sciences. Sponsored by National Inst. of Justice, Washington, DC.

Keywords: *Compandor transmission, Amplitude modulation, Intelligibility, Single sideband transmission, Land mobile radio.

Amplitude companded sideband (ACSB) has been proposed as a useful technique for the land mobile communications needed by law enforcement agencies. These users have certain requirements that their communications systems must meet in order for them to be effective; one of these requirements is for adequate speech intelligibility under a variety of conditions. The report describes the basic principles of operation and those technical aspects of ACSB that may affect speech quality, and then, proposes a measurement program to determine what performance measures are appropriate to characterize the aspect of ACSB performance. It is assumed that the intelligibility of an FM system operating at the condition of 12 dB SINAD represents a reference level of intelligibility. The measurement program will attempt to determine, using the articulation score (AS), the values of the chosen performance measures for ACSB that correspond to the reference level of intelligibility.

*600,687*
**PB86-197209** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Electronic Bulletin Boards,**
T. Landberg. Apr 86, 38p NBSIR-86/3356

Keywords: Information systems, Computer applications, *Electronic message systems.

Many organizations have established electronic bulletin boards to distribute information products electronically. For organizations that need to rapidly distribute press releases, product information, provide customer support or transfer data to a geographically dispersed constituency, electronic bulletin boards are proving to be an inexpensive solution. Bulletin board software is a highly specialized application designed to accomplish a rather limited function of peer to peer communication. Each feature of a bulletin board has been developed to accomplish a different aspect of peer to peer communication. These features include sending and receiving messages, transferring files, and chatting with the system operator. However, bulletin board systems cannot search a textual data base by keyword, initiate other computer jobs or create and edit new data files.

*600,688*
**PB86-203015** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.
**GRIDNET: A Highly Survivable Digital Communications Network. Final Report, Phase 1,**
A. Mink, G. G. Nacht, A. L. Koenig, and A. W. Holt. Apr 86, 33p NBSIR-86/3361
Sponsored by Defense Nuclear Agency, Washington, DC.

Keywords: *Pulse communication, Survival, Optical communication, Fiber optics, Computer systems programs, *Packet switched networks, Packet switching, Protocols, Wide area networks.

GRIDNET is a highly reliable and survivable packet switched, wide area communication network that may consist of thousands of nodes and may span thousands of miles. The reliability of GRIDNET is based on redundant transmission of data via two distinct paths and bitwise comparison of the duplicate received data in addition to error detection codes. The survivability of GRIDNET is attributed to its intrinsic topology, which provides for a number of alternative paths between pairs of nodes. A feasibility prototype of a GRIDNET was proposed as a multi-phase research project. The report describes the design of the phase I GRIDNET prototype which was constructed. This prototype satisfied all of the Phase I operational performance objectives.

*600,689*
**PB87-105185** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Optical Fiber Power Meters: A Round Robin Test of Uncertainty.**
Final rept.,
R. L. Gallawa, and S. Yang. 1986, 3p
Pub. in Applied Optics 25, n7 p1066-1068, 1 Apr 86.

Keywords: *Power meters, *Fiber optics, Optical communication, Detectors, Errors, Reprints, *Optical fibers, Uncertainty, Intercomparison.

The proliferation of optical fiber systems has spawned a variety of optical power meters. These meters are important to the analysis and maintenance of fiber communication systems. One obvious attendant concern is with the uncertainty of the meter readings. In the paper, the authors give the results of an interlaboratory test conducted to circumscribe and define the extent of the problem. The test yielded 46 data points from 11 participants collected over a period of about 9 months. The results indicate that the variation in power meter readings taken in different laboratories is unreasonably large. The variance improved when measurements taken with very small detectors were excluded from the data base. This suggests that errors are being made in the collection of power in typical laboratory environments.

*600,690*
**PB87-108668** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Use of Mode Transfer Matrices in L.A.N. (Local Area Network) Loss Evaluation.**
Final rept.,
J. M. Maisonneuve, P. Churoux, and R. L. Gallawa. 1985, 4p
Pub. in SPIE Fiber Optics: Short-Haul and Long-Haul Measurements and Applications II 559, p182-185 1985.

Keywords: *Fiber optics, Reprints, *Local area networks, Mode transfer matrices.

A method, using Mode Transfer Matrices (MTM) to characterize step index fiber components and predict Local Area Network (LAN) power budget, is presented. The results show this method is well adapted to describing modal power distribution variations.

*600,691*
**PB87-131322** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Calibration Requirements for EHF Satellite Communication Systems,**
R. C. Baird, W. C. Daywitt, A. C. Newell, S. Perera, and A. G. Repjar. Oct 86, 39p NBSIR-86/3058
Prepared in cooperation with CyberLink Corp., Boulder, CO. Sponsored by Air Force Satellite Control Facility, Sunnyvale, CA.

Keywords: *Spacecraft communication, Millimeter waves, Atmospheric attenuation, Extremely high frequencies, *Calibration, MILSTAR system.

The calibration and measurement support requirements of millimeter wave satellite systems such as MILSTAR have been investigated. The needs for measurements on satellite systems are reviewed. An overview of the various means available for calibrating antenna gain, one of the key measurements that needs to be accurately accomplished, is presented. Essentially three new measurement problems arise because of operating in the upper SHF and EHF frequency ranges. First, without adequate methods to measure the atmospheric loss, the accuracy of effective isotropic radiated power (EIRP) measurements in the 20-45 GHz range can be no better than 0.5-3 dB (depending on frequency and antenna elevation angle), which is inadequate for MILSTAR requirements. Second, standards and measurement support services are not presently available from the National Bureau of Standards and are needed to support millimeter wave antenna gain and thermal noise measurements. Third, if the Sun and/or Moon are to be used for measuring Earth terminal G/T, Earth terminal antenna gain, or satellite EIRP in the millimeter region, they need to be appropriately characterized at those frequencies.

*600,692*
**PB87-132247** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.
**Testing to Assure Interworking of Implementations of ISO/OSI (International Organization for Standardization/Open Systems Interconnection) Protocols.**
Final rept.,
R. J. Linn. 1986, 10p
Pub. in Computer Networks 11, n4 p277-286 Apr 86.

Keywords: Standards, Tests, Computer networks, Reprints, *Open systems interconnections, *Communication networks, *ISO/OSI Protocols, Protocols, National Bureau of Standards, International Organization for Standardization, ISO.

At the Institute for Computer Sciences and Technology of the National Bureau of Standards, an architecture has been specified for testing protocols in layers four through seven of the International Organization for Standardization's (ISO) Basic Reference Model for Open Systems Interconnection (OSI). The paper describes the application of that architecture to testing Class 4 Transport with thirteen vendors' implementations of the protocol prior to a demonstration of ISO protocols at the National Computer Conference in 1984. The test results are summarized and an evaluation of the architecture and individual tools is presented. The paper concludes with a summary of a more ambitious demonstration of networking using implementation of ISO protocols.

*600,693*
**PB87-134821** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
**Performance Measurements on the NBS (National Bureau of Standards) Local Data Test Network.**
Final rept.,
D. S. Grubb. 1984, 7p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Global Telecommunications Conference, GLOBECOM '84: Communications in the Information Age, Atlanta, GA., November 26-29 1984, p859-865.

Keywords: *Computer networks, Interfaces, Standards, Input output routines, *Communication networks, *Local Data Test network, *LDTN network, *Data communication protocol, Mainframe computers, Minicomputers, Computer performance evaluation, National Bureau of Standards.

The report describes data communication performance measurements made on the Local Data Test Network (LDTN) at the National Bureau of Standards. The network is an implementation of a network proposed as an American National Standard by Task Group 5 on Future Interfaces of the X3T9 Committee on I/O Interfaces. The proposed network is intended for the connection of mainframe computers and large mini-computers to each other and to their input/output subsystems.

## Graphics

*600,694*
**AD-A147 500/3** PC **A07**/MF **A01**
Army Armament Research and Development Center, Aberdeen Proving Ground, MD. Ballistic Research Lab.
**Electronic Typesetting Program Programmer's Manual.**
Final rept.,
J. H. Whiteside, and C. G. Messina. Aug 84, 130p
ARBRL-MR-03379, SBI-AD-F300 488
This report supersedes IMr-755, dated October 1982.

Keywords: *Typography, *Electronic equipment, *Photocomposition, Firing tables, Printing equipment, Programming manuals, Artillery, Electronic typesetting.

A new method of processing the data to make print masters (images from which printing plates are made) for artillery firing tables has been developed. The new system uses electronic typesetting, derived from the National Bureau of Standards Typographic System, to prepare data for a photocomposition machine. This is a programmer's manual with information on how the program works, how to alter it to produce artillery firing tables, and the structure of the Typographic System from which it is derived.

*600,695*
**PB87-140281** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Tiletool: A Graphical Interface for the Exploration of Generalized Penrose Tilings,**
S. Ressler. Nov 86, 18p NBSIR-86/3488
Sponsored by Bureau of Engraving and Printing, Washington, DC.

Keywords: *Printing, *Printing papers, *Security, Engraving, Interfaces, Bond papers, *Computer graphics.

A graphical system to experiment with non-periodic tilings of a plane has been developed. Non-periodic tilings have several properties which may be useful in the domain of security printing. A large variety of visually interesting patterns which conform to the constraint of non-periodicity may be rapidly produced with the system. The interaction has been made usable by organizing a set of flexible, consistent, and redundant mechanisms for the selection and modification of the various parameters.

## Policies, Regulations, & Studies

*600,696*
**AD-P004 572/4** PC **A02**/MF **A01**
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**New Time and Frequency Services at the National Bureau of Standards,**
S. R. Stein, G. Kamas, and D. W. Allan. 2 Apr 84, 11p
Pub. in Proceedings of the Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (15th) Held at Washington, DC on 6-8 December 1983, AD-A149 163, p17-27.

Keywords: *Time standards, Measurement, Calibration, Accuracy, Precision, Global positioning system, Component Reports, National Bureau of Standards.

The two new measurement services offered in 1983 extend the range and capability of the other frequency and time services offered by NBS: telephone time of day; high frequency broadcasts (WWV and WWVH); low frequency broadcast (WWVB), the GOES satellite time code; and laboratory calibrations. These services previously provided routine time synchronization capability in the one second to 25 microsecond range. The new services offer enhanced automation and a greater confidence in the results of the measurements. In addition, NBS provides consultation to assist the user in selecting the best solution to his problems, initial training and follow-up consultation whenever measurement problems are detected. The new time and frequency services provide traceability to NBS and a direct link to one of the world's best time scales. They greatly reduce the need for the user to become an expert on the intracacies of navigation systems such as Loran-C and GPS. The systems reliability will be high because all the components are off-the-shelf commercial equipment and because NBS maintains the systems to minimize hardware failures.

*600,697*
**PB84-155571** PC **A06**/MF **A01**
National Bureau of Standards, Washington, DC.
**American National Standard X3.102 User Reference Manual,**
N. B. Seitz, and D. S. Grubb. Oct 83, 107p NTIA-REPORT-83-125

Keywords: *Telecommunication, *Standards, Data transmission, Manuals.

American National Standard X3.102 defines a set of 21 standard parameters that provide a uniform means of specifying the performance of data communication systems and services as seen by users. This report is basically an explanation and elaboration of that standard. The report first outlines the benefits of using the standard from the viewpoint of the end user, the communication provider, and the communication manager. The report then summarizes the standard's overall approach and content in informal, non-technical terms. Finally, the report examines the meaning and importance of each standard parameter in a series of tutorial parameter descriptions. Typical parameter values are presented and their design implications are discussed.

*600,698*
**PB86-238664** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Recent Trends in NBS (National Bureau of Standards) Time and Frequency-Distribution Services.**
Final rept.,
R. E. Beehler, and D. W. Allan. 1986, 3p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) 74, n1 p155-157 1986.

Keywords: *Time signals, *Frequency distribution, Radio broadcasting.

Since 1967 the National Bureau of Standards has improved its traditional radio broadcast services from WWV, WWVH, and WWVB and introduced several new services to meet changing needs. The new services are described briefly, including the GOES satellite time code, the Frequency Measurement Service using Loran-C and WWVB, and the Global Time Service based on the GPS satellite common-view technique.

*600,699*
**PB87-122529** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Time Scale Stabilities Based on Time and Frequency Kalman Filters.**
Final rept.,
J. A. Barnes, and D. W. Allan. 1985, 6p
Pub. in Proceedings of Annual Symposium on Frequency Control (39th), Philadelphia, PA., May 29-31, 1985, p107-112.

Keywords: *Frequency control, Frequency stability, *Kalman filters.

The paper details the various scale performances between measurements and provides an insight into the different performances based on computer simulation studies. For example, the 'Time' Kalman filter displays discrete steps in the time corrections where the 'Frequency' Kalman filters are continuous (being the integral of a bounded process). Depending on whether one is most interested in minimizing the RMS time error or minimizing the Allan Variance, one chooses the one time scale over the other.

*600,700*
**PB87-122537** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**New System for Measuring Frequency.**
Final rept.,
G. Kamas, and M. Lombardi. 1985, 7p
Pub. in Proceedings of National Conference of Standards Laboratories 1985 Workshop and Symposium, Boulder, CO., July 15-18, 1985, p224-231.

Keywords: *Frequency measurement.

The paper provides an overview of the NBS Frequency Measurement Service. It begins by discussing the basis for the new service, and the equipment supplied with the service. It shows the advantages of the output data obtained with the service. It explains how the system works and discusses accuracy, reliability, and ease of use. The paper also discusses how the NBS supports the service with training, on-line diagnostics, published measurement data, and monthly performance reports.

*600,701*
**PB87-134938** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**High-Accuracy Global Time and Frequency Transfer with a Space-Borne Hydrogen Maser Clock.**
Final rept.,
R. Decher, D. W. Allan, C. O. Alley, C. Baugher, and B. J. Duncan. 1983, 17p
Pub. in Proceedings of Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (14th), Greenbelt, MD., November 30-December 1-2, 1982, p205-221 1983.

Keywords: Frequency standards, *Time transfer, *Frequency transfer, Hydrogen masers, Space shuttles, Global.

The paper describes a proposed system for high-accuracy global time and frequency transfer using a hydrogen maser clock in a space vehicle. Direct frequency transfer with an accuracy of 10 to the -14th power and time transfer with an estimated accuracy of 1 nsec are provided by a 3-link microwave system. A short pulse laser system is included for subnanosecond time transfer and system calibration. The basic concept of such a system was discussed at the 1980 PTTI Meeting. The paper presents the results of further studies including operational aspects, error sources, data flow, system configuration, and implementation requirements for an initial demonstration experiment using the Space Shuttle.

## Radio & Television Equipment

*600,702*
**PB86-232337** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Guide to Base Station Communications Equipment.**
Final rept.,
R. M. Jickling. 1985, 33p
Sponsored by National Inst. of Justice, Washington, DC.
Pub. in NIJ Guide 204-83, 33p 1985.

Keywords: *Radio equipment, Transmitter receivers, Antennas, Law enforcement, Reprints.

The guide presents information to assist the law enforcement community and others in the selection and procurement of base station communications equipment. The effects of propagation, interference and noise on communications are described briefly. Emphasis is placed on the description of commercially available base station equipment, such as transmitters, receivers, antennas, control units and transmission lines. Auxilliary equipment such as power generators, tone-coding systems, voice scramblers and digital systems are described in less detail.

*600,703*
**PB87-121109** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Electromagnetics LAP Handbook: Operational and Technical Requirements of the Laboratory Accreditation Program for Electromagnetics Compatibility and Telecommunications,**
J. Horlick, and H. Berger. Sep 86, 33p NBSIR-86/3447

Keywords: *Telecommunication, *Laboratories, *Electromagnetic compatability, Equipment, Manuals, Tests, Requirements, *Accreditation, Programs.

The document explains the operational and technical requirements of the Laboratory Accreditation Program (LAP) for Electromagnetics Compatibility and Telecommunications (Electromagnetics LAP). All of the steps leading to accreditation are discussed. Technical requirements are explained indicating how the NVLAP criteria are applied. It is intended for use by the staff of accredited laboratories, those seeking accreditation, other laboratory accreditation systems, and others needing information on the requirements for NVLAP accreditation under this LAP.

## General

*600,704*
**PB86-186863** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Bulletin Board System for Feedback to the Durcon Expert System: A Description and Reference,**
L. J. Kaetzel, and J. R. Clifton. Mar 86, 27p NBSIR-86/3332

Keywords: *Telecommunication, Feedback, *Electronic bulletin boards, Computer networks, Electronic message systems.

The electronic communication of information among building research experts through the use of a computer speeds up the feedback process for projects requiring the exchange of ideas. The DURCON expert system requires such feedback in the form of evaluation, suggested changes and the communication of expert knowledge related to the project. The report describes a bulletin board system that has been established to aid the researchers in communicating effectively.

*600,705*
**PB86-193133** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.
**Description of Text Structures Defined for Office Document Interchange.**
Final rept.,
J. E. Knoerdel, and R. Pierce. 1983, 14p
Pub. in Jnl. of Telecommunication Networks 2, n4 p371-384.

Keywords: *Documents, *Office management, Organizations, Telecommunication, Reprints, *Foreign technology.

The paper discusses many issues related to interchanging documents among office systems and some solutions to the problems created in document interchange. Further, it provides a tutorial on the approach to document interchange being taken within the ANSI, ISO, and CCITT standards organizations. That approach entails definition of document architecture as two separate structures, logical structure and layout structure, which are related by use of layout directives. Those architectural components are then represented in an office document interchange format with varying amounts of logical information and layout information. An interchange format which contains only the layout structure is called a text image format (TIF), while one with only the logical structure or a mixture of logical and layout structure is called a text processable format (TPF).

*600,706*
**PB87-135034** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Methodology for Evaluating Microwave Anechoic Chamber Measurements.**
Final rept.,
M. Kanda. 1985, 6p
Pub. in Proceedings of Symposium and Technical Exhibition Electromagnetic Compatibility (6th), Zurich (Switzerland), March 5-7, 1985, p69-74.

Keywords: *Anechoic chambers, Microwave frequencies, Plane waves, Measurement, Evaluation.

The anechoic chamber measurement is evaluated in terms of the net power delivered to a transmitting antenna, the near-zone gains of open-ended rectangular waveguides and rectangular pyramidal horns, and reflections from chamber walls. The on-axis field intensity of the standard transmitting horn in an anechoic chamber is calculated in terms of the net power delivered to the transmitting antenna. The resulting data can be used for estimating the overall uncertainty in the anechoic chamber measurements. The statistical control of the measurement process by use of transfer standard antennas will monitor the measurement uncertainties. The paper discusses the methodology for evaluating anechoic chamber measurements.

# COMPUTERS, CONTROL & INFORMATION THEORY

## Computer Hardware

*600,707*
**FIPS PUB 114** PC **E06**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**200 MM (8 in) Flexible Disk Cartridge Track Format Using Two-Frequency Recording at 6631 BPRAD on One Side - 1.9 TPMM (48 TPI) for Information Interchange. Category: Hardware Standard. Subcategory: Interchange Codes and Media.**
Federal information processing standards (Final),
Michael D. Hogan. c1985, 21p
Prepared in cooperation with International Organization for Standardization, Geneva (Switzerland).
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Electric drives, Data processing equipment, *Flexible disks, Federal information processing standards, Cartridges.

The standard prescribes a set of physical track format specifications for single-sided, single-density, 200 mm (8 in) flexible disk cartridges which have a data density of 6631 bits per radian (bprad) and 77 tracks at a track density of 1.9 tracks per millimeter (tpmm) (48 tracks per inch (tpi)). Citing these specifications will help to

ensure that interchange parties can reliably interchange data files between information processing systems. This standard incorporates by reference (with qualifications as noted) the technical specifications of ISO 5654/2.

*600,708*
**FIPS PUB 115** PC **E07**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**200 MM (8 in) Flexible Disk Cartridge Track Format Using Modified Frequency Modulation Recording at 13262 BPRAD on Two Sides - 1.9 TPMM (48 TPI) for Information Interchange. Category: Hardware Standard. Subcategory: Interchange Codes and Media.**
Federal information processing standards (Final),
M. D. Hogan. c1985, 25p
Prepared in cooperation with International Organization for Standardization, Geneva (Switzerland).
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Electric drives, Data processing equipment, *Flexible disks, Federal information processing standards, Cartridges.

The standard prescribes a set of physical track format specifications for two-sided, double-density, 200 mm (8 in) flexible disk cartridges which have a data density of 13262 bits per radian (bprad) and 77 tracks at a track density of 1.9 tracks per millimeter (tpmm) (48 tracks per inch (tpi)). Citing these specifications will help to ensure that interchange parties can reliably interchange data files between information processing systems. This standard incorporates by reference (with qualifications as noted) the technical specifications of ISO 7065/2.

*600,709*
**FIPS PUB 116** PC **E07**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**130 MM (5.25 in) Flexible Disk Cartridge Track Format Using Two-Frequency Recording at 3979 BPRAD on One Side - 1.9 TPMM (48 TPI) for Information Interchange. Category: Hardware Standard. Subcategory: Interchange Codes and Media.**
Federal information processing standards (Final),
M. D. Hogan. c1985, 23p
Prepared in cooperation with International Organization for Standardization, Geneva (Switzerland).
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Electric drives, Data processing equipment, *Flexible disks, Federal information processing standards, Cartridges.

The standard prescribes a set of physical track format specifications for single-sided, single-density, 130 mm (5.25 in) flexible disk cartridges which have a data density of 3979 bits per radian (bprad) and 35 tracks at a track density of 1.9 tracks per millimeter (tpmm) (48 tracks per inch (tpi)). Citing these specifications will help to ensure that interchange parties can reliably interchange data files between information processing systems. This standard incorporates by reference (with qualifications as noted) the technical specifications of ISO 6596/2.

*600,710*
**FIPS PUB 117** PC **E07**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**130 MM (5.25 In) Flexible Disk Cartridge Track Format Using Modified Frequency Modulation Recording at 7958 BPRAD on Two Sides - 1.9 TPMM (48 TPI) for Information Interchange. Category: Hardware Standard. Subcategory: Interchange Codes and Media.**
Federal information processing standards (Final),
M. D. Hogan. c1985, 22p
Prepared in cooperation with International Organization for Standardization, Geneva (Switzerland).
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Electric drives, Data processing equipment, *Flexible disks, Federal information processing standards, Cartridges.

The standard prescribes a set of physical track format specifications for two-sided, double-density, 130 mm (5.25 in) flexible disk cartridges which have a data density of 7958 bits per radian (bprad) and 40 tracks at a track density of 1.9 tracks per millimeter (tpmm) (48 tracks per inch (tpi)). Citing these specifications will help to ensure that interchange parties can reliably interchange data files between information processing systems. The standard incorporates by reference (with qualifications as noted) the technical specifications of ISO 7487/3.

*600,711*
**FIPS PUB 118** PC **E12**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Flexible Disk Cartridge Labelling and File Structure for Information Interchange. Category: Software Standard. Subcategory: Operating Procedure.**
Federal information processing standards (Final),
M. D. Hogan. c1985, 37p
Prepared in cooperation with International Organization for Standardization, Geneva (Switzerland).
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Electric drives, Data processing equipment, *Flexible disks, Federal information processing standards, Cartridges.

The standard prescribes a set of logical track format specifications for flexible disk cartridges described in the following physical track format standards; FIPS PUB 114, FIPS PUB 115, FIPS PUB 116, and FIPS PUB 117. The standard incorporates by reference (with qualifications as noted) the technical specifications of ISO 7665.

*600,712*
**PB86-164514** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Modeling and Test Point Selection for Data Converter Testing.**
Final rept.,
T. M. Souders, and G. N. Stenbakken. Nov 85, 5p
Sponsored by Institute of Electrical and Electronics Engineers, Inc., New York.
Pub. in Proceedings of International Test Conference, 1985, Philadelphia, PA., November 19-21, 1985, p813-817.

Keywords: *Data converters, Digital to analog converters, Mathematical models, Tests.

Methods for generating efficient testing strategies for data converters are presented. Linear modeling techniques based on circuit analysis and empirical test data are included, as well as algorithms for selecting optimal test points. Using these tools, converter errors can be accurately estimated for all code states from a relatively small number of measurements.

*600,713*
**PB86-203411** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Software Technology Div.
**Planning and Implementing System Reliability.**
Final rept.,
L. S. Rosenthal. 1983, 7p
Pub. in Proceedings of Total Systems Reliability Symposium, Gaithersburg, MD., December 12-14, 1983, p112-118.

Keywords: Systems management, Reliability, Guidelines, *Computer systems design, *Computer program reliability.

The paper is an abbreviated version of a NBS publication of the same name and is part of the Computer System Selection and Evaluation Program within the Bureau's Institute for Computer Sciences and Technology. It is intended to assist the system manager in acquiring a basic understanding of computer system reliability concepts, techniques, and controls.

*600,714*
**PB86-244175** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.
**National Bureau of Standards Workshop on Performance Evaluation of Parallel Computers,**
S. B. Salazar, and C. H. Smith. Jul 86, 51p NBSIR-86/3395

Keywords: *Bench marks, Measurement, Workshops, Laboratories, Universities, Industries, National government, *Parallel computers, *Computer performance evaluation, National Bureau of Standards.

The Systems Components Division of the Institute for Computer Sciences and Technology at the National Bureau of Standards is actively engaged in the development of techniques to measure and evaluate the performance of parallel computers. As a preliminary step, a workshop on performance evaluation was held in Gaithersburg, Maryland on June 5th and 6th, 1985. The goal of the workshop was to define the issues and problems involved in the development of benchmarks for large parallel computers. Thirty-six talks were given by representatives of government, industries, universities and research laboratories. The topics presented ranged from specific measurements of large parallel machines to the philosophical issues concerned with the development of universally applicable benchmarks. The document is a report on the workshop.

*600,715*
**PB87-122776** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
**National Bureau of Standards Research Program for the Archival Lifetime Analysis of Optical Digital Data Disks (O(D sup 3)).**
Final rept.,
S. B. Geller. 1984, 4p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers 490, p80-83 1984.

Keywords: *Life(Durability), *Archives, Data processing, Information retrieval, Drives, Servomechanisms, Lasers, Chemical tests, Physical properties, Dynamic tests, Information systems, *Optical disks, Computer storage management, Failure(Electronics), National Bureau of Standards.

The Institute for Computer Sciences and Technology at the National Bureau of Standards (NBS/ICST) is embarking on a research program into the life expectancy properties of optical digital data disks (OD3). The paper discusses lifetime concepts in a general sense and some philosophies and objectives which will underlie the NBS/ICST archival program when it is initiated. Whereas the associated OD3 systems including optical disk drives, servos, lasers, and optics are usually replaceable (providing that they do not fall into the one-of-a-kind category), data contents which are lost due to the OD3 media failure may be irretrievable. Therefore, the principal archival lifetime factors to be investigated by NBS are related primarily to the life expectancies of the OD3 media and media structures. The initial program efforts will be towards determining the system independent degradation and failure mechanisms of the media materials through static optical, chemical, and physical testing. Subsequently, where possible these static test results will be correlated with the results derived from dynamic tests of the system dependent degradation and failure mechanisms of the media.

## Computer Software

*600,716*
**AD-A147 834/6** PC **A02**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Dialogue Mechanisms in a Tabletop Programming Environment,**
G. Lyon, M. V. Zelkowitz, J. Elgot, D. Itkin, and B. Kowalchack. 20 Sep 84, 10p AFOSR-TR-84-0936
Contract F49620-83-K-0018
Pub. in Proceedings IEEE COMPCON Fall 84, p33-39, 16-20 Sep 84.

Keywords: *Man computer interface, *Integrated systems, *Computer programming, High level languages, Syntax, Microcomputers, Programmers, Editing, User needs, Reprints, Syntax directed editors, Pascal programming language.

No abstract available.

*600,717*
**PB86-162047** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div.

## Computer Software

**Some Experience with Testing Tools for OSI (Open Systems Interconnection) Protocol Implementations.**
Final rept.,
R. J. Linn, and J. S. Nightingale. 1983, 11p
Pub. in Proceedings of the International Workshop on Protocol Specification, Testing, and Verification (3rd), Ruschlikon, Switzerland, May 31-June 2, 1983, p521-531.

Keywords: Verifying, Specifications, Tests, Programming languages, *Foreign technology, *Open systems interconnections, *Federal information processing standards, *Software tools, Computer architecture, Transport protocols.

At the Institute for Computer Sciences and Technology (ICST), test architecture has been specified for testing protocols of layers four through seven within the ISO Basic Reference Model for Open Systems Interconnection. The paper describes specific tools within the test architecture which have been developed and refined using a prototype implementation of the NBS Class 4 Transport Protocol. The language which drives the tool provides the mechanisms to edit protocol data units.

*600,718*
**PB86-162054** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div.
**Producing Tests for Implementations of OSI (Open Systems Interconnection) Protocols.**
Final rept.,
R. J. Linn, and W. H. McCoy. 1983, 16p
Pub. in Proceedings of the International Workshop on Protocol Specification, Testing, and Verification (3rd), Ruschlikon, Switzerland, May 31-June 2, 1983, p505-520.

Keywords: Tests, Design, Computational linguistics, Grammars, *Foreign technology, *Open systems interconnections, Transport protocols, Protocols.

Problems associated with protocol test design, semantics and completeness are explored. A linguistics approach utilizing a generative grammar augmented with probability distributions associated with the production rules and random selection is used to produce test sequences for the NBS/ICST implementation of ISO Class 4 Transport protocol. Advantages and limitations of the methodology are presented.

*600,719*
**PB86-167830** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Integrated Software for Microcomputer Systems.**
Final rept.,
L. S. Rosenthal. Jan 86, 41p NBS/SP-500/135
Also available from Supt. of Docs as SN003-003-02711-1. Library of Congress catalog card no. 86-600500.

Keywords: Microcomputers, *Computer software, *Integrated systems, Application programs(Computers), Operating systems(Computers).

Integrated software products combine several applications within a single program and enable information to be shared between the applications. The report defines five approaches to integration: the all-in-one, product suite, software integrator, operating environment, and background utility. Each of these approaches is designed to achieve different objectives by emphasizing the power and importance of the features of each approach. Consequently, there is no best approach to software integration. The selection of an approach depends on the application requirements, current system configurations, and personal preferences. Selecting an integrated product begins by considering the various approaches to integration and determining which one is most appropriate. Subsequently, the products within the chosen approach are evaluated against a preestablished set of criteria relating to the product design, technical capabilities, and product quality. Careful selection of an integrated product will insure that the benefits to be gained from its use can be achieved.

*600,720*
**PB86-169349** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Computer Science and Technology: An Overview of Computer Software Acceptance Testing.**
Final rept.,
D. R. Wallace. Feb 86, 28p NBS/SP-500/136
Also available from Supt. of Docs as SN003-003-02712-0. Library of Congress catalog card no. 86-600502.

Keywords: Acceptability, Tests, Proving, Planning, Guidelines, *Computer software, *Computer program verification, Validation, User needs.

The document provides guidance in planning and managing acceptance testing of computer software. It emphasizes the need for quantitative acceptance criteria and itemized test cases and procedures. It provides a checklist of activities to be performed for planning and managing acceptance testing.

*600,721*
**PB86-185295** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.
**Testing OSI (Open System Interconnection) Protocols: NBS (National Bureau of Standards) Advances the State of the Art.**
Final rept.,
K. L. Mills. Mar 84, 9p
Pub. in Data Communications 13, n3 p277-285 Mar 84.

Keywords: *Computer networks, Automation, Tests, Reprints, *Open system interconnections, Protocols.

The Institute for Computer Sciences and Technology (ICST) has established a methodology and architecture for testing implementations of standard open systems interconnection protocols. The ICST has also developed a set of automated tools to support the testing of protocols. The document describes the methodology, architecture, and test tools; provides a summary of experience to date; and outlines future plans for testing implementation of standard open system interconnection protocols.

*600,722*
**PB86-186855** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.
**Performance Measurement Techniques for Multiprocessor Computers.**
Interim rept.,
J. W. Roberts. Feb 86, 59p NBSIR-85/3296
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.

Keywords: Performance, Measurement, *Multiprocessors, *Computer performance evaluation.

A wide range of possible measures for multiprocessor computers is discussed, along with the realizability of each class of measurement technique and the applicability of the results.

*600,723*
**PB86-189099** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.
**Generating Artificial Traffic Over a Local Area Network Using Random Number Generators.**
Final rept.,
L. A. Ramshaw, and P. D. Amer. 1983, 19p
Pub. in Computer Networks 7, n4 p233-251 Aug 83.

Keywords: Algorithms, Random numbers, Generators, Traffic, Sequencing, Reprints, *Local area networks, *Computer performance evaluation.

Effective testing and performance evaluation of a local area computer network requires the ability to generate artifical traffic. This in turn requires algorithms for generating random number sequences. The article evaluates several random number generation algorithms considered for emulating traffic over NBSNET, a local area computer network at the National Bureau of Standards. The table-based method, using an additive uniform random number generator for selection from the table, was determined to be a satisfactory method considering NBSNET's constraints, and is being used to generate artificial traffic for continuing local network research experimentation.

*600,724*
**PB86-196482** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Software Engineering Project Standards.**
Final rept.,
M. A. Branstad, and P. B. Powell. 1984, 6p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Software Engineering SE-10, n1 p73-78 Jan 84.

Keywords: *Standards, Reprints, *Software engineering, *Computer software.

Software Engineering Project Standards (SEPS) and their importance are presented in the article by looking at standards in general, then progressively narrowing the view to software standards, to software engineering standards, and finally to SEPS. After defining SEPS, issues associated with the selection, support, and use of SEPS are examined. A brief overview of existing software engineering standards is presented and trends are discussed.

*600,725*
**PB86-202066** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Software Requirements Analysis: A Disciplined Approach.**
Final rept.,
P. B. Powell. 1983, 2p
Sponsored by Institute of Electrical and Electronics Engineers, Inc., Piscataway, NJ. Service Center.
Pub. in Proceedings of the International Computer Software and Applications - COMPSAC 83 Conference (7th), Chicago, Illinois, November 7-11, 1983, p642-643.

Keywords: Quality, Requirements, *Software engineering, *Computer program reliability, Software tools, Analysis.

The paper addresses software requirements analysis from a management point of view with the goal of producing software requirements which are complete, consistent, and unambiguous. Three type of analysis are mentioned, static, dynamic and formal, to promote a disciplined approach to requirements analysis. Among the benefits which can be derived from this approach are confidence raising that the requirements are complete and consistent, improving the quality of the software, and promoting reliability.

*600,726*
**PB86-203437** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Performance and Cost Characterization of A-Tree (Real-Time) Hashing (Extended Abstract).**
Final rept.,
G. Lyon. 1983, 1p
Sponsored by Johns Hopkins Univ., Baltimore, MD.
Pub. in Proceedings of Annual Conference on Information Sciences and Systems (17th), Baltimore, MD., March 23-25, 1983, p477.

Keywords: *Search structuring, *Data retrieval, *Addressing, Tables(Data), Searching, Algorithms, Performance, *Memory devices, Computer software, Access time, Real time, Cost.

Hashing is a software realization of content-addressable memory. Average hash retrievals are swift but worst cases, especially failed-lookups, are often unacceptably slow. Yet open-addressing hasing with mild restrictions can limit all searches to two probes: Attractive as this may be, available construction methods have been computation-bound and impractical. A new, fast algorithm--a-tree hashing--builds the open-addressing tables in times linear with their size. In descending importance, design objectives for the a-tree hash table builder are: incremental open-addressing insertion; searching in one or two probes; economical table construction; good average retrieval; easy coding; light memory demands.

*600,727*
**PB86-203445** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Need for Management of Software Maintenance.**
Final rept.,
R. J. Martin. 1983, 2p
Sponsored by Computer Society (IEEE), Los Alamitos, CA.
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) International Computer Soft-

ware and Applications Conference (7th), COMPSAC 83, Chicago, IL., November 7-11, 1983, p83-84.

Keywords: Management, Guidelines, *Software maintenance, Software engineering.

The paper develops the thesis that a software maintenance manager must not only be a good maintainer, but also a good manager. It presents an overview of some of the key findings of a National Bureau of Standards' Institute for Computer Sciences and Technology project to investigate and develop guidance on software maintenance.

*600,728*
**PB86-203452** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Controlling Software Change.**
Final rept.,
W. M. Osborne. 1983, 3p
Sponsored by Computer Society (IEEE), Los Alamitos, CA.
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Computer Society's International Computer Software and Applications Conference (7th), COMPSAC 83, Chicago, IL., November 7-11, 1983, p89-90.

Keywords: Computer software, *Software maintenance, Software engineering, User needs.

The paper addresses three issues necessary for controlling software change: centralized approval, formal requests, and involvement of the user, management, and maintenance staff in the maintenance change process.

*600,729*
**PB86-214236** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Software Technology Div.
**Reconstituting Shared Variables.**
Final rept.,
G. Lyon. 1982, 1p
Pub. in Proceedings of Conference on Information Sciences and Systems, Princeton, NJ., March 17-19, 1982, p246.

Keywords: *Computer programming, *Binary digits, *Machine coding, Abandonment, Bits, Variables.

In expanding the efficiency and flexibility of variables shared among tasks, it is not uncommon to allow 'read-lock' as a variable state. Once this accommodation is made, there are three states: unlocked, read-locked, and write-locked. Since two bits allow four possible states, a fourth value-abandoned-can be introduced. 'Abandoned' is then assigned whenever a task owning a write-locked variable terminates abnormally. A problem arises because recovery of abandoned shared variables can engender problems in writing secure, error-free programs. Addressing this not unimportant facet, the idea will be to diminish chances of abandoned objects (variables) slipping into unlocked status through programming error or oversight.

*600,730*
**PB86-214244** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Software Technology Div.
**Considerations for Effective Program Development Systems.**
Final rept.,
P. Henderson, and G. Lyon. 1982, 6p
Pub. in Proceedings of Conference on Information Sciences and Systems, Princeton, NJ., March 17-19, 1982, p247-252.

Keywords: *Editing routines, *Interpreters, Microcomputers, Computer systems programs, Productivity, Programmers, *Software engineering, *Software tools.

The explosive push of microcomputers will render many computational services almost free. Accordingly, there exists an excellent opportunity for improving the productivity of programmers, while at the same time enhancing the quality of the programs produced. One component of a microprocessor based software development system is an interactive program constructor-executor similar to, but more powerful than, a BASIC editor-interpreter. Our purpose here is to (i) give a brief survey of characteristics of existing constructor-executor systems; (ii) to discuss a spectrum of useful enhancements to the characteristics of such systems.

*600,731*
**PB86-229622** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Functional Model for Fourth Generation Languages.**
Final rept.,
G. E. Fisher. Jun 86, 40p NBS/SP-500/138
Also available from Supt. of Docs as SN003-003-02731-6. Library of Congress catalog card no. 86-600545.

Keywords: *Programming languages, Data processing, Services, *Fourth generation programming languages, *Computer software, Data management, High level languages, On line systems, User needs, Applications programs(Computers).

The Fourth Generation Language (4GL) functional model places 4GL in the context of programming language evolution, and describes the functions provided within the context. A 4GL is a software system that provides integrated functions for developing interactive on-line data processing applications. These functions are defined as: (1) user functions that define those services and capabilities necessary to provide a high level dialogue between the 4GL and users of the 4GL; (2) data management functions that provide capabilities to describe, store and retrieve, and perform ancillary tasks in the management and safekeeping of application data; and (3) system functions that provide the support services necessary to allow the user of 4GL to define and access applications in relation to the constraints of the 4GL's environment. A typical implementation of 4GL distributes pieces of these functions over various components, such as a DBMS, query language, data dictionary, screen formatter, report generator, and high level procedural language.

*600,732*
**PB86-231420** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
**Mathematical Software in Basic: RV, Generation of Uniform and Normal Random Variables.**
Final rept.,
D. Kahaner, J. Horlick, and D. Foer. Jun 86, 9p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Micro 6, n3 p52-60 Jun 86.

Keywords: *Random numbers, Basic programming language, Reprints, Computer applications.

Two programs, written in Basic, are described for generating uniform and normal random numbers.

*600,733*
**PB86-232329** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Information Systems Engineering Div.
**Reference Models for Standardization.**
Final rept.,
E. N. Fong, and D. K. Jefferson. 1986, 5p
Pub. in Proceedings of Computer Standards Conference, 1986-Striking a Balance between Technology, Economics, Politics, and Reality - For Substance, Not Form, San Francisco, CA., May 13-15, 1986, p86-90.

Keywords: *Standards, *Standardization, Development, Methodology, Protocols, Programming languages, *Data base management systems, Computer graphics, Computer communications, Reference model, Software engineering.

As the use of computer technology becomes more complex and pervasive, computer standards are being developed to facilitate the interconnection of components and transfer of programs, data, and skills from one environment to another. There are standards activities in the areas of programming languages, database management systems, computer communication protocols, graphics, and software engineering. Since these standards may overlap or interact with one another, there is a need for 'standard' methods to help manage the development of standards. One such method is to use a 'reference model' (RM) for an area in which standards are to be developed. A RM is a conceptual framework which divides standardization work into manageable pieces, and shows, at a general level, how these pieces are related to each other.

*600,734*
**PB86-232352** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Computer Security Evaluation and Certification.**
Final rept.,
Z. G. Ruthberg. 1982, 9p
Sponsored by Department of Defense, Washington, DC.
Pub. in Proceedings of Seminar on DOD Computer Security Initiative (5th), Gaithersburg, MD., May 24-26, 1982, p207-215.

Keywords: Security, Classified matter, Evaluation, Guidelines, *Computer security, Certification.

The paper is based on a talk given at the Fifth Conference of the Department of Defense Computer Security Initiative, May 24-26, 1982. It initially, presents a brief history of the certification and evaluation efforts at ICST/NBS and definitions of the centrally important terms 'computer security', 'computer security evaluation', 'security certification', 'computer system', 'computer application', and 'sensitive application'. It then goes on to briefly describe the certification and evaluation projects at ICST/NBS.

*600,735*
**PB86-232360** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Computer Security and Risk Management Program.**
Final rept.,
S. W. Katzke. 1982, 10p
Sponsored by Department of Defense, Washington, DC.
Pub. in Proceedings of Seminar on DOD Computer Security Initiative (5th), Gaithersburg, MD., May 24-26, 1982, p157-166.

Keywords: *Data processing security, Technical assistance, *Computer security, *Computer information security, Data encryption, Federal agencies, Risk analysis.

ICST/NBS has a computer security and risk management (CSRM) program that provides technical assistance to Federal agencies in reducing ADP related risks. The article discusses the scope of the Computer Security problem, Federal agencies' responsibilities for providing CSRM, and ICST's CSRM program objectives and activities designed to assist Federal agencies in meeting their responsibilities.

*600,736*
**PB86-245263** PC **A02**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Study of a Prototype Software Engineering Environment,**
D. R. Wallace, and D. R. Kuhn. Jun 86, 24p NBSIR-86/3408

Keywords: Prototypes, Environments, *Software engineering, *Software tools, Federal agencies, User needs.

A prototype software engineering environment was studied as part of the program to provide information to Federal agencies on software tools for improving quality and productivity in software development and maintenance. The purpose of a software engineering environment is to surround its users with software tools necessary for systematic development and maintenance of software. The report presents the results of the study of the prototype software engineering environment with respect to its features. The report also presents several factors to consider when evaluating a software engineering environment.

*600,737*
**PB86-247590** PC **A02**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Experiment in Software Acceptance Testing,**
D. R. Wallace. Jul 86, 20p NBSIR-86/3407

Keywords: Acceptability, Prototypes, Productivity, *Software engineering, *Software tools, *Software quality control, Federal agencies.

Software acceptance testing was performed on a prototype software engineering environment as part of the program to provide information to Federal agencies for improving quality and productivity in software development and maintenance. The purpose of software acceptance testing is to demonstrate to its purchasers that the software satisfies its requirements. The report

describes the method and standards applied in this study in software acceptance testing. The report also discusses the difficulties encountered during the study and proposes research directions for software acceptance testing.

*600,738*
**PB87-108551** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Guide to the Selection and Use of Fourth Generation Languages.**
Special pub. (Final),
M. M. Gray. Sep 86, 70p NBS/SP-500/143
Also available from Supt. of Docs as SN003-003-02758-8. Library of Congress catalog card no. 86-600582.

Keywords: *Programming languages, *Fourth Generation programming languages, *High level languages, End use.

The report provides guidance on the selection process for Fourth Generation Languages (4GLs). It also gives a description of the features, functions and capabilities of 4GLs; and a brief discussion on the use of 4GLs. A ten step selection process is suggested: (1) describing the application; (2) analyzing the application environment; (3) deciding on selection approach; (4) defining requirements; (5) developing list of desired 4GL features; (6) rating desired features; (7) selecting candidate packages; (8) rating 4GLs; (9) analyzing top few in detail; and (10) selecting 4GL. Check lists are provided for screening 4GLs and analyzing the application environment.

*600,739*
**PB87-109849** PC **A07**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Annotated Bibliography on Software Maintenance,**
W. M. Osborne, and R. Raigrodski. Sep 86, 142p NBS/SP-500/141
See also PB87-109856. Also available from Supt. of Docs as SN003-003-02756-1. Library of Congress catalog card no. 86-600579.

Keywords: *Bibliographies, Maintenance, Productivity, Errors, Measurement, Technical reports, Periodicals, *Software maintenance, Computer software, Software tools, Software configuration management, Software quality control, Life-cycle cost, Cost, User needs.

The annotated bibliography contains summaries of two hundred and eighty-five software maintenance articles or papers from computer science journals, books, proceedings, Federal publications, computer newspapers, and other technical reports. It covers a fifteen year period between 1972 and 1986, and presents an overview of the various aspects of software maintenance including problems and issues faced in most software maintenance environments. It identifies techniques, procedures, methodologies, and tools that have been effectively employed throughout the software system lifecycle to improve the quality of that system.

*600,740*
**PB87-109856** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Management Overview of Software Reuse,**
W. Wong. Sep 86, 27p NBS/SP-500/142
See also PB87-109849. Also available from Supt. of Docs as SN003-003-02757-0. Library of Congress catalog card no. 86-600581.

Keywords: Organizations, Management, Productivity, Economic analysis, *Reusable software, *Software engineering, Software quality control, Costs.

With skyrocketing software costs, both Federal and private sector organizations are increasingly interested in finding ways to improve software quality and productivity, and reduce software risks: Software reuse is one promising method of accomplishing the objective. The report presents a management overview of the problems and issues related to software reuse. It provides a description of software reusability and its scope. The necessity of technical and management involvement to achieve greater levels of software reuse is emphasized.

*600,741*
**PB87-122669** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**SETKY-GETKY, Keyed Access System for the HP1000.**
Final rept.,
D. Bickham, and D. Neumann. 1986, 16p
Pub. in Proceedings of Conference on INTEREX International Association of Hewlett-Packard Computer Users, Detroit, MI., September 28-October 3, 1986, p1-16.

Keywords: Data processing, Data files, Data displays, Data bases, Information retrieval, Data storage, Chemistry, *Access methods, *HP1000 computers, *SETK-GETKY system, Computer output devices, On line systems, User manuals(computer programs), Formats, User needs, Minicomputers.

SETKY-GETKY is a keyed access system written for the HP1000 mini-computer. Its main function is to provide rapid access to free formatted textual or tabular material stored in large data files. It provides a choice among output devices and some user control over the format of the data display. Three examples are presented to demonstrate the use of SETKY-GETKY. The first is a simple example of a database of computer users. The second example shows the development of an online help system and user's manual. The last example involves the storage and retrieval of tables of chemical thermodynamic functions.

*600,742*
**PB87-140810** PC **A06**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Guidance on Software Package Selection.**
Final rept.,
S. Frankel. Nov 86, 124p NBS/SP-500/144
Also available from Supt. of Docs as SN003-003-02773-1. Library of Congress catalog card no. 86-600593.

Keywords: Evaluation, Guidelines, *Computer software, *Applications program(Computers).

The report describes a systematic procedure for identifying and evaluating off-the-shelf software packages, and for incorporating the selected package into the organizational environment. Its purpose is to enable the layperson to choose and implement software packages with a minimum of dependence on technical personnel. The report provides guidance on each phase of the package selection and implementation process.

## Control Systems & Control Theory

*600,743*
**PB86-196268** CP **T03**
National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.
**Hierarchical Control System Emulator Version 3.2.**
Model,
C. Furlani. Apr 86, mag tape NBS/SW/MT-86/006
Supersedes PB85-233823.
Source tape is in the ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. Call NTIS Computer Products if you have questions. Price includes documentation, PB85-233849, PB85-233831 and PB83-175075.

Keywords: *Models-simulation, *Control simulation, *Automatic control, Computerized simulation, Magnetic tapes, Real time operations, Industrial plants, Production control, Automation, Fortran, *Hierarchical control, *Control systems, *Computerized control systems, *Computer aided design, Computer aided manufacturing, Emulators(Computers), Praxis programming language, VAX-11/780 computers.

The Hierarchical Control System Emulator is a collection of computer programs written in the high-level Praxis language for use on a Digital Equipment Company VAX/780 processor under the VMS operating system. These programs allow the user to write, debug, and concurrently emulate modules of a hierarchical control system and to simulate the physical plant which is controlled. The emulation executes in real time and interactive display and data logging capabilities are included. The emulator is currently implemented at the NBS Automated Manufacturing Research Facility as a computer-aided control system design tool. The magnetic tape contains a copy of version 3.2 of the entire HCSE software package. In addition, the tape is accompanied by an instruction sheet which describes the procedure for transferring the HCSE from magnetic tape to a VAX/VMS system...Software Description: The model is written in the FORTRAN programming language for implementation a Digital VAX-11/780 computer using the VAX/VMS operating system.

## Information Processing Standards

*600,744*
**FIPS PUB 104-1** PC **A02**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**American National Standard Codes for the Representation of Names of Countries, Dependencies, and Areas of Special Sovereignty for Information Interchange. Category: Data Standards and Guidelines. Subcategory: Representations and Codes.**
Federal information processing standards (Final),
R. G. Saltman. 12 May 86, 25p
Three ring vinyl FIPS binder also available, North American Continent price $6.25; all others write for quote

Keywords: *Geography, *Standards, Information, Exchanging, Data, Dependence, *Federal information processing standards, Nations, Sovereignty, Alphanumeric data, Codes, Information processing.

The Federal Program Standard implements American National Standard ANSI Z39.27-1984, Structure for the Representation of Names of Countries, Dependencies, and Areas of Special Sovereignty for Information Interchange. ANSI Z39.27 adopts, with qualifications, the entities, names, and codes prescribed by ISO 3166-1981, Codes for the Representation of Names of Countries, a standard of the International Organization for Standardization (ISO). The qualifications provide for coverage of the total land area of the earth without overlap or duplication, and provide for entity names that, to the maximum extent possible, are approved or accepted by the U.S. Board on Geographic Names. Both two-character and three-character alphabetic codes are provided for each entity adopted from ISO 3166-1981. The two-character codes are adopted as the Federal Program Standard and they are recommended by ISO for international interchange. The three-character codes are available for special applications when their use would provide a particular advantage.

*600,745*
**FIPS PUB 112** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Password Usage. Category: ADP Operations. Subcategory: Computer Security.**
Federal information processing standards (Final),
D. K. Branstad. 30 May 85, 60p
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: Data processing, Identification systems, Authentication, Guidelines, *Federal information processing standards, *Computer security, *Data processing security, *Password, Access, Managers.

The document specifies basic security criteria for two different uses of passwords in an ADP system, (1) personal identity authentication and (2) data access authorization. It establishes the basic criteria for the design, implementation and use of a password system in those systems where passwords are used. It identifies fundamental ADP management functions pertaining to passwords and specifies some user actions required to satisfy these functions. In addition, it specifies several technical features which may be implemented in an ADP system in order to support a password system. An implementation schedule is established for compliance with the Standard. Numerous guidelines are provided in the Appendices for managers and users seeking to comply with the Standard.

*600,746*
**FIPS PUB 120** PC **E13**
National Bureau of Standards, Gaithersburg, MD.

**Graphical Kernel System (GKS). Category: Software Standard. Subcategory: Graphics.**
Federal information processing standards (Final),
D. R. Benigni. c1985, 400p
Prepared in cooperation with American National Standards Inst., New York.
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Computer graphics, *Federal information processing standards, *Graphical kernel system, *Software tools, *Computer program portability.

The publication announces the adoption of the American National Standard Graphical Kernel System (ANS GKS), ANSI X3.124-1985, as a Federal Information Processing Standard (FIPS). ANS GKS specifies a library (or toolbox package) of subroutines for an application programmer to incorporate within a program in order to produce and manipulate two-dimensional pictures. The purpose of the standard is to promote portability of graphics application programs between different installations. The standard is for use by implementors as the reference authority in developing graphics software systems; and by other computer professionals who need to know the precise syntactic and semantic rules of the standard.

*600,747*
**FIPS PUB 121** PC **E06**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Videotex/Teletext Presentation Level Protocol Syntax (North American PLPS). Category: Hardware and Software Standard. Subcategory: Interchange Codes.**
Federal information processing standards (Final),
J. L. Little. c1983, 181p
Prepared in cooperation with American National Standards Inst., New York.
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Television systems, Standards, *Federal information processing standards, *Open systems interconnections, *Video networks, Presentation layer protocols.

The standard describes the formats, rules, and procedures for the encoding of alphanumeric text and pictorial information for videotex and teletext applications. It is based upon the architecture defined in the multi-layered reference model of open systems interconnection (OSI), under development by the ISO, and defines a specific data syntax for use by OSI presentation layer protocols and some specific semantics for use at the application layer. Based upon ASCII and its extensions (as specified in FIPS 1-2), it adopts the whole American National Standard X3.110-1983/Canadian Standard T500-1983, Videotex/Teletext Presentation Level Protocol Syntax (North American PLPS). It is intended to be used in Federal information processing systems, communications systems, and associated videotex/teletext equipment.

*600,748*
**FIPS PUB 122** PC **E05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Conformance Tests for FIPS PUB 100/FED-STD 1041 Version of CCITT 1980 Recommendation X.25, Interface between Data Terminal Equipment (DTE) and Data Circuit-Terminating Equipment (DCE) for Operation with Packet-Switched Data Communications Networks. Category: Conformance Tests.**
Final rept.,
M. K. Wong. 28 May 86, 211p
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Interfaces, *Data processing terminals, Computer networks, Telecommunication, *Federal information processing standards, *Communtican networks, X-25 protocol, Packet switching, Communication terminals.

The document describes a set of verification tests designed by the Institute for Computer Sciences and Technology (ICST) at the National Bureau of Standards (NBS) to evaluate the conformance to the joint Federal Information Processing Standard Publication 100 (FIPS PUB 100)/Federal Standard 1041 (FED-STD 1041) for the interface to an X.25 packet switched network. A fundamental objective of these verification tests is concerned with establishing uniform verification testing and unambiguous evaluation procedures to aid government users in acquiring ADP and telecommunications facilities or services based on the X.25 specifications. These tests are designed for use by vendors and suppliers so as to provide government users with assurance the products they acquire are in conformance with the FIPS PUB 100/FED-STD 1041 specifications and can interwork.

*600,749*
**FIPS PUB 123** PC **E04**
National Bureau of Standards, Gaithersburg, MD.
**Specification for a Data Descriptive File for Information Interchange (DDF). Category: Software Standard. Subcategory: Information Interchange.**
Federal information processing standards (Final),
J. V. Upperman. 19 Sep 86, 43p
Three ring vinyl binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Standards, *Data transmission, *Information systems, Specifications, Computer networks, *Files(Records), *Federal Information Processing Standards, *Data conversion, *Information transfer, Data structures, Formats, Communications networks, Computer software.

The publication announces the adoption of the ANSI/ISO 8211-1985, Specification for a Data Descriptive File for Inforamtion Interchange (DDF), as a Federal Information Processing Standard (FIPS). ANSI/ISO 8211-1985 specifies media-independent and system-independent file and record formats for the interchange of information between computer systems. The standard is intended for use with physical media as well as with communications media in applications where a high volume of data is to be interchanged, rather than for an isolated interchange of a single or small number of resources. The purpose of the standard is to provide a mechanism to allow data structures to be easily transported from one computer system to another computer system, independent of make, with the capability of restructuring the data without loss of who have a need to represent data structures and data definitions in a standard format for information interchange purposes so that the data can be transported from one system to another while maintaining the integrity of the data.

*600,750*
**FIPS PUB 69-1** PC **E13**
National Bureau of Standards, Gaithersburg, MD.
**FORTRAN. Category: Software Standard. Subcategory: Programming Language.**
Federal information processing standards.
c1985, 464p
Supersedes FIPS PUB 69.
Three ring vinyl FIPS binder also available, North American Continent price $6.25; all others write for quote.

Keywords: *Fortran, *Standards, Documents, Data processing, National government, Programming languages, *Federal information processing standards, *Software engineering, *Computer program portability.

The publication announces the revision of Federal Information Processing Standard FORTRAN. The revision supersedes FIPS PUB 69 and reflects changes to the Objectives, Applicability, and Implementation portions of FIPS FORTRAN. FIPS FORTRAN is the adoption of American National Standard Programming Language FORTRAN, X3.9-1978. The American National Standard specifies the form and establishes the interpretation of programs expressed in the FORTRAN programming language. The standard consists of a full language and a subset language. The purpose of the standard is to promote portability of FORTRAN programs for use on a variety of data processing systems. The standard is used by implementors as the reference authority in developing compilers, interpreters, or other forms of high level language processors, and by other computer professionals who need to know the precise syntactic and semantic rules of the standard.

*600,751*
**PB86-203429** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
**Software Engineering Standards: Motives and Mechanisms.**
Final rept.,
M. Branstad. 1983, 4p
Proceedings of Software Engineering Standards Application Workshop (2nd), San Francisco, CA., May 17-19, 1983, p83-86.

Keywords: *Standards, Groups, Workshops, *Software engineering.

In recent years there has been an increased interest in software engineering (SWE) standards. Many groups are establishing standards, often as apparently independent activities. The paper discusses standards in general and software engineering standards in particular, the groups who are developing software engineering standards, the needs that drive their standardization efforts, and the forces that influence and constrain the standards.

*600,752*
**PB86-232097** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
**New Computer-Based Self-Correcting Calibration System for Computer Storage Media Standard Reference Materials.**
Final rept.,
F. L. Podio. 1985, 6p
Pub. in Computers and Standards 4, n4 p231-236 1985.

Keywords: *Computer storage devices, *Magnetic tapes, *Standards, Calibrating, Automatic control, Self organizing systems, Reprints, National Bureau of Standards.

A new method for calibrating magnetic computer storage media Standard Reference Materials (SRMs) has been developed at the National Bureau of Standards (NBS). The calibration system applies to a new class of higher density Standard Reference Magnetic Computer Storage Media. The foundation of the method is based on both the analysis of and experience with the present well-established SRM calibration systems. Errors that would be introduced into the calibration process by unwanted system changes are prevented from doing so through the use of self-correcting techniques.

*600,753*
**PB86-232311** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Information Systems Engineering Div.
**Emerging Software Standards: Opportunity and Challenge.**
Final rept.,
H. M. Wood. 1986, 5p
Pub. in Proceedings of Computer Standards Conference, 1986-Striking a Balance between Technology, Economics, Politics, and Reality - For Substance, Not Form, San Francisco, CA., May 13-15, 1986, p122-126.

Keywords: *Standards, Vendors, Competition, Utilization, *Computer industry, *Information transfer, Computer software, International Organization for Standardization, User needs.

Although computer technology standards have been under development for over two decades, all too often the results of these activities were overlooked or underutilized. Now users are faced with differing proprietary products that inhibit transfer of information. Meanwhile, the U.S. computer industry is facing increased international competition, coupled with the threat of a variety of restrictive national standards. As a result, the demand for communications and software standards has surged--not only from users, but from vendors as well. Fortunately, a number of needed standards are flowing out of national and international standards organizations to meet the demand. The paper will consider emerging software standards and efforts to speed their development and use.

*600,754*
**PB87-128286** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.
**Testing OSI (Open Systems Interconnection) Protocols at the National Bureau of Standards.**
Final rept.,
R. J. Linn, and J. S. Nightingale. 1983, 4p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) 71, n12 p1431-1434 Dec 83.

Keywords: Tests, Protocols, Programming languages, *Open systems interconnections, *Federal information processing standards, National Bureau of Standards.

## Information Processing Standards

The Institute for Computer Sciences and Technology at the National Bureau of Standards has developed an architecture for testing implementations of OSI protocols, to establish conformance with the appropriate Federal Information Processing Standards. The paper gives a justification for specific design choices made, describes architectural elements and gives an example of a test language used to drive the test system.

*600,755*
**PB87-142436** CP **T05**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Codes for Named Populated Places, Primary County Divisions, and other Locational Entities of the United States (FIPS PUB 55), 9th Update.**
Data file.
1 Dec 86, mag tape NBS/DF/MT-87/003
Supersedes PB86-154002.
Data file is available in the EBCDIC and ASCII character sets on 9-track one-half inch tape. Identify recording mode by specifying density and character set. Call NTIS Computer Products if you have questions.

Keywords: *Data file, *Populations, *Coding, *States(United States), Urban areas, Communities, Magnetic tapes, *Federal Information Processing Standards, *Population distributions, *Geographic areas, *Standard metropolitan statistical areas, *Counties, Computer applications.

The ninth update of the Federal Information Processing Standard (FIPS) 55 data file provides a two-character State code and five-character numeric place code to uniquely identify each listed entity. Areas of the United States covered are the fifty States, the District of Columbia, and all outlying territories with significant self-administration. An exhaustive list is carried of incorporated places, census designated places (CDP's), primary county divisions (such as townships, New England towns, and census county divisions), recognized Indian reservations and Alaska native villages and counties. The listing also includes unincorporated places, military bases, National parks, airports, and ground transportation points. A two-character class code distinguishes over seventy entity types. Each entity is identified by the county or counties in which it is located. All exhaustive categories and military bases are identified by Congressional (99th) District and by all new metropolitan statistical areas. Incorporated places, CDP's and Indian and Alaska native areas, are cross-referenced to U.S. Bureau of the Census files. ZIP codes are provided for all post offices.

## Pattern Recognition & Image Processing

*600,756*
**PATENT-4 601 055** Not available NTIS
Department of Commerce, Washington, DC.
**Image Processor.**
Patent,
E. W. Kent. Filed 10 Apr 84, patented 15 Jul 86, 24p
PB86-221843, PAT-APPL-6-598 602
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Patents, *Display devices, Television cameras, Robots, Mapping, *Image processing, PAT-CL-382-49, Computer applications.

An iconic-to-iconic low-level image processor is provided which comprises a plurality of identical sequential intermediate stages located between an input stage adapted to be connected to image sources such as analog or digital television cameras, ranging devices and conformal mapping arrays and an output stage adapted to be connected, e.g. to monitors, robot vision systems, iconic symbolic mapping devices and image processing computers. The intermediate stages are provided with forward pathway connections which afford sequential image processing as well as retrograde (feedback) pathway connections between adjacent stages in reverse sequence and within stage, recursive pathway connections for each stage. The stages each include neighborhood operators and image buffers and a number of operations are supported including neighborhood operations on images within each stage and between-stage operations on each pixel such as threshold, boolean and arithmetic operations, function mappings and the like.

*600,757*
**PB86-241940** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Image Quality Indicators.**
Final rept.,
D. Polansky. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v3 p2263-2265 1986.

Keywords: *Images, Quality, Reprints.

No abstract available.

*600,758*
**PB87-131843** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**PIPE (Pipelined Image Processing Engine).**
Final rept.,
E. W. Kent, M. O. Shneier, and R. Lumia. 1985, 29p
Pub. in J. Parallel Distrib. Comput. 2, n1 p50-78 Feb 85.

Keywords: Reprints, *Image processing, Computer vision, *PIPE(Pipelined Image Processing Engine).

The Sensory-Interactive Robotics Group of the National Bureau of Standards' Industrial Systems Division is designing and constructing an experimental multistage pipelined image processing device for research in machine vision. The device can acquire images from a variety of sources, such as analog or digital television cameras, ranging devices, and conformal mapping arrays. It can process sequences of images in real time, through a serial pipeline of operations, under the control of an external device. Its output can be presented to such devices as monitors, robot vision systems, iconic to symbolic mapping devices, and image processing computers. In addition to a forward flow of images through successive stages of operations in the pipeline, other paths between the stages of the device can permit recursive operations within a single stage, and feedback of the results of operation from a stage to the preceding stage. The architecture facilitates a variety of relaxation operations, interactions of images over time, and other interesting functions. Numerous operations can be supported.

*600,759*
**PB87-132239** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Design and Function of the NBS (National Bureau of Standards) Pipelined Image Processing Engine.**
Final rept.,
E. W. Kent, M. O. Shneier, and R. Lumia. 1985, 18p
Pub. in Proceedings of Conference on Vision '85, Detroit, MI., March 25-28, 1985, p8.40-8.57.

Keywords: *Robots, Mapping, Arrays, Television cameras, Feedback, *Image processing, *Robot vision, *Parallel processing, Real time, National Bureau of Standards.

The Sensory-Interactive Robotics Group of the National Bureau of Standards is producing PIPE (Pipelined Image Processing Engine), an experimental, multistage, multi-pipelined image processing device for research in low-level machine vision. The device can acquire images from a variety of source, such as analog or digital television cameras, ranging devices, and conformal mapping arrays. It can process sequences of images in real time, through a series of local neighborhood and point operations, under the control of a host device. Its output can be presented to such devices as monitors, robot vision systems, iconic to symbolic mapping devices, and image processing computers.

## General

*600,760*
**PB85-161040** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Security of Personal Computer Systems: A Management Guide.**
Final rept.,
D. D. Steinauer. Jan 85, 66p NBS/SP-500/120
Also available from Supt. of Docs as SN003-003-02627-1. Library of Congress catalog card no. 84-601156.

Keywords: Guidelines, *Personal computers, *Computer security, *Computer information security, Home computers, Cryptography, Office automation, Access control.

This document is a security guide for managers and users of personal computer systems. It describes the nature of information security problems involved in the use of personal and other small computer systems and provides guidance for addressing those problems.

*600,761*
**PB86-202579** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div.
**Evaluation of the ICST (Institute for Computer Sciences and Technology) Test Architecture after Testing Class 4 Transport.**
Final rept.,
R. J. Linn. 1985, 11p
Pub. in Proceedings of the IFIP WG 6.1 International Workshop on Protocol Specification, Testing, and Verification (4th). Skytop Lodge, PA., June 11-14, 1984. p611-621 1985.

Keywords: *Computers, *Architecture, Tests, *Protocols, *Computer networks.

At the Institute for Computer Sciences and Technology of the National Bureau of Standards, an architecture has been specified for testing protocols in layers four through seven of the ISO Basic Reference Model for Open Systems Interconnection. The paper describes the application of that test architecture to testing Class 4 Transport with thirteen vendors' implementations of the protocol. The test results are summarized and an evaluation of the architecture and individual tools are presented.

*600,762*
**PB86-202587** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div.
**Use of ISO Class 4 Transport on Local Area Networks.**
Final rept.,
D. P. Stokesberry. 1983, 13p
Pub. in Proceedings of LOCALNET '83, Local Networks, Distributed Office and Factory Systems, New York, NY., June 27-29, 1983, p371-383.

Keywords: Computers, *Computer networks, *Local area networks, *Computer communications, Protocols.

At the request of a number of companies, the National Bureau of Standards has organized three workshops for local area computer network implementors to arrange a multi-vendor demonstration of ISO Class 4 Transport Protocol on local area networks that implement the IEEE 802 protocols. Eighty-nine people from 45 organizations attended at least one of the workshops. The participants agreed to establish two neutral sites to demonstrate the ISO Transport and IEEE 802 local area network protocols. One site, hosted by General Motors, will support the IEEE P-802.4 Token Bus local area network standard. The second site, hosted by NBS, will support the IEEE P-802.3 CSMA/CD standard. Both sites will implement IEEE P-802.2 type 1, class 1 logical link control service for layer 2, an octet of zero representing a null network independent convergence protocol for layer 3 and the mandatory portions of the NBS specification of ISO Class 4 transport for layer 4.

*600,763*
**PB86-202595** Not available NTIS
National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div.
**Characterization of Traffic on NBSNET.**
Final rept.,
D. P. Stokesberry. 1984, 40p
Pub. in Proceedings of a Workshop on Performance and Evaluation of Local Area Networks, Worcester, MA., March 24-25, 1983, p63-102 1984.

Keywords: *Computers, *Communication traffic, *Computer networks, *Local area networks, *Computer communications, Protocols.

The paper analyzes the traffic on a local area network in its third year of operation at the National Bureau of Standards. NBSNET is a one megabit per second broadcast network that uses a carrier sense multiple access with collision detection (CSMA/CD) protocol. It is approximately four kilometers in length. The network has over 250 user devices connected to it; these devices fall into six different categories -- main computer, minicomputer, microcomputer, word processor, graphics terminal and ordinary terminal. Over 2 million packets were observed during 39 data collection runs. One fourth of the packets and one third of the data are local, i.e., the source address and the destination address of the packets are located in the same building. The rest of the traffic is between buildings. The network is growing continuously and network traffic increases as the network grows.

*600,764*
**PB86-213097** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Security for Dial-Up Lines.**
Special pub. (Final),
E. F. Troy. May 86, 68p NBS/SP-500/137
Also available from Supt. of Docs as SN003-003-02723-5. Library of Congress catalog card no. 86-600531.

Keywords: *Data processing security, *Authentication, Dials, Modems, Telephone lines, Display devices, Computer system hardware, *Computer privacy, *Computer information security, *Computer security, *Data processing security, *Secure communications.

The publication describes a set of solutions to the problem of intrusion into government and private computers via dial-up telephone lines, the so-called 'hacker problem'. There are a number of minimum protection techniques against these people and more nefarious intruders that should be used in all systems that have dial-up communications. These techniques can usually be provided by a computer's operating system. If the computer, augmented by normal security procedures, does not have the capability to give adequate protection against dial-up intruders, then additional software or hardware should be used to shore up the system's access control security. There are several types of hardware devices which can be fitted to computers or used with their dial-up terminals to provide additional communications protection for non-classified computer systems.

*600,765*
**PB86-231172** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
**Using DES (Data Encryption Standard) in IBM PC Compatible Workstations.**
Final rept.,
M. E. Smid. 1986, 9p
Pub. in Proceedings of 1986 IEEE (Institute of Electrical and Electronics Engineers) Workstation Technology and Systems Conference, Atlantic City, NJ., March 17-20, 1986, p1-9, Supplement.

Keywords: *Data processing security, Standards, Algorithms, Compatability, *Cryptography, *Data encryption, Workstations, IBM PC computers, Personal computers.

The Data Encryption Standard (DES) cryptographic algorithm can be implemented in International Business Machines Corporation (IBM) PC compatible workstations to protect data from unauthorized disclosure and to detect unauthorized modifications. Commercial products are now available, or will soon be available, to perform the required cryptographic processing. System designers should consider several issues, including the following: what applications tasks are to be performed, which cryptographic processes are needed, what configuration is best for the required tasks, what requirements will be placed upon the system by the connected networks, how will cryptographic keys be managed, and which standards should be met by the cryptographic equipment.

*600,766*
**PB86-247897** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Work Priority Scheme for EDP (Electronic Data Processing) Audit and Computer Security Review,**
Z. G. Ruthberg, and B. T. Fisher. Jul 86, 61p NBSIR-86/3386
Prepared in cooperation with Department of Health and Human Services, Washington, DC. Office of the Inspector General.

Keywords: *Auditing, *Information systems, Reviews, Efficiency, *Risk analysis, *Computer security, *Computer information security, Priorities, Work measurement.

The report describes a high level risk analysis for Automated Information Systems (AISs) that can be used by computer security reviewers and EDP auditors to prioritize their non-discretionary and discretionary review activities for these AISs. It divides the risk analysis problem into five areas of risk concern (called dimensions) with each area defined by a set of characteristics. The five dimensions are: Criticality/Mission Impact, Size/Scale/Complexity, Environment/Stability, Reliability/Integrity, and Technology Integration. The report presents a possible two-level scoring scheme which calculates the level of risk for each dimension, uses the Criticality score as a first order system risk score, and then combines all five dimension risk scores for a second order system risk score. An approach for deriving an EDP audit or computer security review plan using these scores is outlined.

# ELECTROTECHNOLOGY

## Antennas

*600,767*
**PB86-160140** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Array of Dipoles for Plane Wave Synthesis.**
Final rept.,
D. A. Hill, and G. H. Koepke. Aug 85, 4p
Sponsored by Commemorative Association for the Japan World Exposition.
Pub. in Proceedings of the International Symposium on Antennas and Propagation (1985), Kyoto, Japan, August 20-22, 1985, p177-180.

Keywords: *Plane waves, *Dipole antennas, *Dipoles, *Phased arrays, Electromagnetic fields, Synthesis, Near fields.

Phased arrays can be used to produce a nearly uniform plane wave in the near field. The paper describes a small array of dipoles which we have studied theoretically and experimentally. The element excitations are determined from a near-field synthesis technique that optimizes the field uniformity throughout the test volume.

*600,768*
**PB86-162021** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Measured Vehicular Antenna Performance.**
Final rept.,
R. L. Jesch. May 85, 11p
Pub. in IEEE (Institute of Electrical and Electronic Engineers) Transactions on Vehicular Technology VT-34, n2 p97-107 May 85.

Keywords: *Ground vehicle antennas, *Amplification, *Antenna radiation patterns, Power gain, Frequencies, Field tests, Reprints.

Power gain radiation patterns of mobile antennas mounted in six different locations on a test vehicle were measured with and without typical lights and sirens mounted on the roof. The measurements were performed at frequencies representing the frequency bands of 25 to 50, 150 to 174, 400 to 512, and 806 to 866 MHz. In addition, special antennas consisting of three disguised antennas operating at discrete frequencies of 40.27, 162.475, and 415.975 MHz and one slot antenna operating at 413 MHz were also measured. Plots of power gain radiation patterns are given for the mobile antennas mounted in six different locations on the test vehicle and for the special antennas. Results showing the effects of poor grounding characteristics are also included. Recommended locations for mounting the mobile antennas are given for specific frequency bands.

*600,769*
**PB86-181963** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Efficient and Accurate Method for Calculating and Representing Power Density in the Near-Zone of Microwave Antennas,**
R. L. Lewis, and A. C. Newell. Dec 85, 44p NBSIR-85/3036

Keywords: *Microwave antennas, *Field strength, Antennas, Electromagnetic fields, Power spectra, Apertures, Algorithms, Near field, Fresnel zone.

An algorithm is presented for calculating near-zone and Fresnel-region fields in front of microwave antennas from discrete numerical values of the radiated plane-wave spectrum (complex far-field pattern). That is, the near fields are calculated by numerically integrating the plane-wave spectrum representation of the field. The crux of the analysis consists of handing a numerical instability which arises from integrating discrete data. A criterion is developed for limiting the integration domain in order to exclude highly oscillatory regions of the integrand. In turn, this leads to restricting the applicable output range over which the field can be computed. With the numerical instability problem thus resolved, fast Fourier transform techniques are used to assure efficient numerical integration over a large (but restricted) output range.

*600,770*
**PB86-189214** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Input Impedance of a Probe Antenna in a TEM (Transverse Electromagnetic) Cell.**
Final rept.,
P. F. Wilson, D. C. Chang, and M. T. Ma. 1984, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electromagnetic Compatibility, EMC-26 n4 p154-161 Nov 84.

Keywords: *Input impedance, *Antennas, Waveguides, Reprints, *Transverse electromagnetic cell.

The input impedance of a probe antenna exciting a transverse electromagnetic (TEM) cell is formulated via a variational approach. The resulting impedance is shown to consist of two distinct terms; an ordinary rectangular waveguide contribution and a gap perturbation. Numerical results for both are given and suggest that a simple algebraic approximation for the input impedance should normally suffice. The resistive portion is found to be proportional to the square of the probe length, while the reactive portion is largely capacitive.

*600,771*
**PB86-214731** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Factors Influencing Material Shielding Effectiveness Measurements.**
Final rept.,
P. F. Wilson, and M. T. Ma. Aug 85, 5p
Pub. in Proceedings of IEEE International Symposium on Electromagnetic Compatibility, Wakefield, MA., August 20-22, 1985, p29-33.

Keywords: *Antennas, *Insertion loss, *Shielding, Electromagnetic shielding.

A material's shielding effectiveness is often measured in terms of insertion loss; that is, the field reduction between a transmitter and receiver achieved by introducing the shield material. The insertion loss concept is simply stated; however, ambiguities arise when one attempts to interpret specific insertion loss measurements. Insertion loss data depend not only on the shield material tested, but also on the measurement procedure. The antenna types used and their positioning, the incident waveform and its wave impedance, and the contact resistance between the test material and its mount (if any) can all affect insertion loss measurements, sometimes dramatically. These concepts are discussed based on the simple model of coupling through an electrically small aperture, loaded and unloaded, with the shield material.

## Antennas

*600,772*
**PB86-230034** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**10-60 GHz G/T Measurements Using the Sun as a Source--A Preliminary Study.**
Rept. for 1985-86,
W. C. Daywitt. Apr 86, 22p NBSIR-86/3046
Sponsored by Air Force Satellite Control Facility, Sunnyvale, CA.

Keywords: *Microwave antennas, *Solar radio emission, Microwaves, Atmospheric attenuation, Sun, Error analysis, Correction, Electromagnetic noise, Amplification, Atmospheric correction, Earth terminal measurement system, G/T.

Preliminary studies show that it may be possible (1) to determine the solar flux density incident on the earth's atmosphere using a simple algorithm with an uncertainty less than 8 percent; (2) to overcome a deteriorating accuracy in atmospheric loss calculations by using a 'tipping curve' measurement, and (3) to reduce star-shape correction factor uncertainty by using an equivalent solar diameter.

*600,773*
**PB86-231438** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Receiving Antenna as a Linear Differential Operator: Application to Spherical Near-Field Scanning.**
Final rept.,
R. C. Wittmann, and A. R. Yaghjian. 1985, 11p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Antennas and Propagation AP33, n11 p1175-1185 Nov 85.

Keywords: *Antennas, Electromagnetic fields, Measurement, Scanning, Reprints, *Near field.

The general receiving antenna is represented as a linear differential operator converting the incident field and its spatial derivatives at a single point in space to an output voltage. The differential operator is specified explicitly in terms of the multipole coefficients of the antenna's complex receiving pattern. When the linear operator representation is applied to the special probes used in spherical near-field measurements, a probe-corrected spherical transmission formula is revealed that retains the form, applicability, and simplicity of the nonprobe-corrected equations. The new spherical transmission formula is shown to be consistent with the previous transmission formula derived from the rotational and translational addition theorems for spherical waves.

*600,774*
**PB86-237203** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Interelement Interactions in Phased Arrays: Theory, Methods of Data Analysis, and Theoretical Simulations.**
Technical note,
L. A. Muth. Dec 85, 50p NBS/TN-1091
Also available from Supt. of Docs. as SN003-003-02715-4.

Keywords: *Phased arrays, Antenna radiation patterns, Interactions, Reflection, Impedance.

The authors review theoretically the effects of multiple reflections and mutual impedances in array environments and study possible methods of far-field pattern data analysis to recover interaction effects. The authors use theoretical expressions derived earlier to calculate in a two-element linear array the mutual-impedance matrix and effective excitations of elements as functions of interelement separation and n sub max, the maximum mode number in the radiation pattern of the elements. Generalizations to two- and three-dimensional arrays are discussed.

*600,775*
**PB86-247491** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Linear Gain - Standard Antennas Below 1000 MHz.**
Technical note,
R. G. FitzGerrell. May 86, 43p NBS/TN-1098
Also available from Supt. of Docs as SN003-003-02736-7.

Keywords: *Antennas, *Amplification, Standards, Ultrahigh frequencies, High f frequencies, Very high frequencies, High frequencies, Medium frequencies.

Gain and antenna parameters related to input impedance are calculated using a computer program called HVD6. The program uses well documented equations to compute these parameters for gain-standard antennas used in relative-gain or gain-transfer measurements at frequencies below 1000 MHz. The utility of the program is that it calculates gain patterns and input impedances for linear dipoles above perfect or imperfectly conducting plane ground and in free space, and for monopoles on perfectly conducting plane ground. Examples are included to illustrate the use of the program. Uncertainties in the calculated parameters are estimated to be less than those of the measured parameters.

*600,776*
**PB87-106407** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Numerical Method for Near-Field Array Synthesis.**
Final rept.,
D. A. Hill. 1985, 11p
Pub. in IEEE Transactions on Electromagnetic Compatibility EMC-27, n4 p201-211 Nov 85.

Keywords: *Phase arrays, Antennas, Electromagnetic fields, Numerical analysis, Plane waves, Reprints, Near field.

A numerical method for near-field array synthesis is developed for arbitrary array geometries. The intended application is for generating a planar field in a test volume for electromagnetic susceptibility testing, but the method is valid for arbitrary field distributions. A uniqueness theorem is utilized to allow the field conditions to be enforced on the surface of the test volume rather than throughout the volume. The synthesis method is a least-squares solution with a constraint on the source norm; the constraint keeps the field small outside the test volume. Numerical results are shown for the case of synthesizing a plane wave in the near field of an array of line sources.

*600,777*
**PB87-125746** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Out-of-Band Response of Antenna Arrays,**
D. A. Hill, and M. H. Francis. Jun 86, 37p NBSIR-86/3047
Sponsored by Defense Nuclear Agency, Washington, DC.

Keywords: *Antenna arrays, Orientation, Impedance matching, Polarization, Near field, Slotted waveguides, Out of band.

The response of antenna arrays to out-of-band frequencies has been analyzed using the effective aperture approach. An average value of effective aperture can be obtained by averaging the incidence angle and the polarization of the incidence field. Far-field patterns have also been calculated by treating the array element excitations as random variables. The randomness in the element excitations causes a decrease in directivity and an increase in sidelobe level. Out-of-band measurements of reflection coefficient and near-field response have been made on two large slotted-waveguide arrays for frequencies from 2 to 18 GHz. Both arrays are narrow band, and this is easily explained by the large impedance mismatch at out-of-band frequencies.

*600,778*
**PB87-134375** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Displacement Errors in Antenna Near-Field Measurements and Their Effect on the Far Field,**
L. A Muth. Oct 86, 38p NBS/TN-1306
Also available from Supt. of Docs as SN003-003-02776-6.

Keywords: *Antenna radiation patterns, Error analysis, Far field, Electrical measurement, Near field.

The effects of probe displacement errors in the near-field measurement procedure on the far-field spectrum are studied. Expressions are derived for the displacement error functions that maximize the fractional error in the spectrum both for the on-axis and off-axis directions. Planar x-y and z-displacement errors are studied first and, consequently, the results are generalized to errors in spherical scanning. Some simple near-field models are used to obtain order of magnitude estimates for the fractional error as a function of relevant scale lengths of the near field, defined as the lengths over which significant variations occur.

## Circuits

*600,779*
**AD-A123 554/8** PC **A02**/MF **A01**
National Bureau of Standards, Washington, DC.
**Microwave Mixing and Direct Detection Using SIS and SIS' Quasiparticle Tunnel Junctions,**
A. D. Smith, W. R. McGrath, P. L. Richards, R. E. Harris, and F. L. Lloyd. 30 Nov 82, 4p
Contract N00014-75-C-0496
Presented at the Applied Superconductivity Conference (1982). Prepared in cooperation with National Bureau of Standards, Boulder, CO. and Yale Univ., New Haven, CT.
Pub. in IEEE Trans. Magn. MAG-19, n3 p490-493 May 1983.

Keywords: *Microwave amplifiers, *Mixers(Electronics), *Tunneling(Electronics), *Junctions, Quantum electronics, Coupling(Interaction), Gain, Detectors, Superconductors, Leakage(Electrical), Microwave mixing, Quasiparticles.

Quasiparticle mixers have shown strong quantum effects, conversion gain, and noise levels approaching the quantum limit, but only in tunnel junctions with very low sub-gap 'leakage' conductance. It has been suggested that SIS' tunnel junctions, made from two different coductors with unequal gaps, will function as high gain mixers since the dynamic conductance below the gap is nagative.

*600,780*
**PB86-160686** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Wide-Band Transconductance Amplifier for Current Calibrations.**
Final rept.,
O. B. Laug. 1985, 5p
Pub. in IEEE (Institute of Electrical and Electronic Engineers) Transactions on Instrumentation and Measurement IM-34, n4 p639-643 Dec 85.

Keywords: *Current amplifiers, *Transconductance, Calibrating, Electric currents, Phase measurement, Reprints.

A wide-band transconductance amplifier for current calibrations is described. The amplifier will deliver a ground-referenced constant current of 5 A rms from dc to over 100 kHz. Its stable magnitude and phase permit it to be used in precise power calibration systems to provide the current component of a phantom power source. The amplifier also provides a ground-referenced voltage output of 1 V/A for monitoring the magnitude and phase of the output current.

*600,781*
**PB86-202991** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**Automated Measurement of Frequency Response of Frequency-Modulated Generators Using the Bessel Null Method.**
J. R. Major, E. M. Livingston, and R. T. Adair. Mar 86, 34p NBS/TN-1093
Also available from Supt. of Docs as SN003-003-02728-6. Sponsored by Army Communications-Electronics Command, Fort Monmouth, NJ.

Keywords: *Signal generators, *Frequency response, Frequency modulation, Measurement, Remote control, Measuring instruments, Bessel null.

The paper describes a Bessel null technique to measure the frequency response of a frequency-modulated rf carrier and a program to automate frequency response measurements of signal generators with output frequencies from 0.450 to 2000 MHz. The measurements obtained using the technique are more precise than those obtained by a highly trained technician using a manual system. Automated measurement of the process is desirable since the manual method is subject to the following problems: (1) excessive time, (2) error in finding the null, and (3) lack of assurance that the null is the first Bessel null. Automated measurements can be performed using a system controller,

a spectrum analyzer, a function generator, and a voltmeter (all of which must be compatible and controllable remotely).

*600,782*
**PB86-229796** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Broad-Band RF Match to a Millimeter-Wave SIS Quasi-Particle Mixer.**
Final rept.,
A. V. Raisanen, W. R. McGrath, P. L. Richards, and F. L. Lloyd. 1985, 6p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Microwave Theory and Techniques MTT-33, n12 p1495-1500 Dec 85.

Keywords: *Mixing circuits, Josephson junctions, Superconductivity, Millimeter waves, Radio astronomy, Reprints.

An integrated superconducting microstrip is shown to be a convenient, flexible, and well-characterized matching element for a super-conductor-insulator-superconductor (SIS) quasi-particle heterodyne mixer. The resonant interaction (Fiske modes) between the Josephson oscillations of a voltage-biased junction and the microstrip provides a convenient method for determining the electrical length of the microstrip line. An open-circuited microstrip stub that reflects a parallel inductance across the junction is used to broaden the bandwidth of the RF match of a 30-40-GHz SIS mixer. Measurements with Pb-alloy junctions in a full-height waveguide mixer with fixed mechanical tuning give an instantaneous bandwidth of 10 to 15 percent with a mixer noise temperature (T sub M) (DSB) = 10 + or - 2.5 K.

*600,783*
**PB86-242005** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Multiport Network Analyzers.**
Final rept.,
C. A. Hoer. 1986, 4p
Pub. in McGraw-Hill Yearbook of Science and Technology, p289-292 1986.

Keywords: *Network analyzers, Reprints.

The paper is a tutorial summary of the principles of multiport network analyzers, their use in microwave measurements of reflection coefficient and scattering parameters, and the significance of this development for the field of microwave measurements.

*600,784*
**PB87-106381** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Efficient Antialiasing Filter.**
Final rept.,
R. A. Lawton. 1985, 4p
Pub. in IEEE Transactions on Instrumentation and Measurement IM-34, n4 p570-573 Dec 85.

Keywords: *Electric filters, Waveforms, Measurement, Solid state devices, Reprints, Time domain.

The application of a solid-state reference filter as an efficient antialiasing filter is described. The analytical basis for the efficiency of the filter is described and a specific example of measuring a 1024-point waveform with an RC filter and the solid-state filter is given.

*600,785*
**PB87-122321** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Surge Suppressors and Clamps.**
Final rept.,
F. D. Martzloff. 1986, 7p
Pub. in Proceedings of EMC EXPO 86 International Conference on Electromagnetic Compatibility, Washington, DC., June 16-19, 1986, pE01.1-E01.7.

Keywords: *Circuit protection, Avalanche diodes, Varistors, *Surge suppressors, Transients.

The paper presents a review of technologies developed for surge suppressor devices used in electronic circuits. Three generic types are described: crowbars, varistors, and avalanche diodes. The significant differences in their performance characteristics are pointed out, with guidance on proper application and measurements.

## Electromechanical Devices

*600,786*
**PB86-231453** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Standardization of Coaxial Connectors in the IEC (International Electrotechnical Commission).**
Final rept.,
N. J. Sladek, and R. L. Jesch. 1986, 5p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Special Issue on Radio Measurement Methods and Standards 74, n1 p14-18 Jan 86.

Keywords: *Electric connectors, Coaxial cables, Standards, Standardization.

The paper reviews the requirements and standardization of coaxial connectors within the International Electrotechnical Commission (IEC) Subcommittee SC46D 'Connectors for RF Cables'. A list of published IEC connector standards and a list of IEC standards under consideration are included.

*600,787*
**PB87-110243** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Errors in Servo Systems Using Sinusoidal Frequency (Phase) Modulation.**
Final rept.,
F. L. Walls. 1986, 5p
Sponsored by Naval Research Lab., Washington, DC.
Pub. in Proceedings of Annual Symposium on Frequency Control (39th), Philadelphia, PA., May 29-31, 1985, p91-95.

Keywords: *Servomotors, Errors, Phase modulation, Frequency modulation.

The paper reviews the errors in determining the center of a resonance line which are due to residual imperfections in practical electronic systems using sinosoidal frequency or phase modulation. In particular the effects of residual amplitude modulation, baseline distortion, and harmonic distortion in the modulation process and the demodulator are qualitatively analyzed for a Lorentzian line in the limit of small modulation index. This permits one to easily calculate analytically the frequency offsets as a function of modulation index and the transfer function of the fundamental and various harmonics of the modulation frequency. Using this model one can easily formulate accurate tests for experimentally measuring the frequency errors in practical servo systems, even if the original assumptions about small modulation index and a pure Lorentzian line are not exactly fulfilled.

*600,788*
**PB87-116174** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Survey of Triaxial and Mode-Stirred Techniques for Measuring the Shielding Effectiveness of Connectors and Cables,**
R. L. Jesch. Oct 86, 24p NBSIR-86/3060
Sponsored by Army Aviation Systems Command, St. Louis, MO.

Keywords: *Shielding, *Transmission lines, *Electric connectors, Connectors, Electrical faults, Tests, Triaxial tests, Effectiveness, Mode stirred techniques.

The report is the result of an extensive literature search conducted in the field of connectors and cables, and of the problem dealing with radio frequency leakage characteristics and the ability to measure the shielding effectiveness of these connectors and cables. It reviews two measurement techniques for determining the shielding effectiveness: the triaxial test technique that has been used for over 20 years and the mode-stirred test technique that recently has started to gain in popularity. From the survey, certain inferences are drawn about these techniques in terms of device configuration, frequency range, and ease of measurement and are presented in chart form for comparative purposes.

## Optoelectronic Devices & Systems

*600,789*
**PB86-183555** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Low-Level Germanium Detector Transfer Standard at 1.064 Micrometers,**
A. L. Rasmussen, and D. L. Franzen. Jan 86, 15p NBSIR-85/3041
Sponsored by Aerospace Guidance and Metrology Center, Newark AFS, OH.

Keywords: *Infrared detectors, *Photodiodes, *Calibrating, *Standards, Near infrared radiation, Light pulses, Germanium, *Transfer standards, Laser radiation, YAG lasers, Light emitting diodes.

Two germanium PIN photodiodes have been calibrated in the 1 to 250 fj/sq cm range with 15 percent uncertainty for 1.064 micrometer laser pulses of 10 to 100 ns duration. To do these calibrations, the authors used (1) an acousto-optically modulated cw Nd:YAG laser beam and a silicon PIN photodiode transfer standard to provide low-level laser pulses of known energy and (2) a pulsed micrometer LED beam. A I sq cm collecting lens and a ground glass diffuser were placed in front of each detector to improve sensitivity and spatial uniformity, respectively. In the future, these detectors may also be useful as transfer standards at wavelengths out to 1.7 micrometers.

*600,790*
**PB86-195567** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Diamond Opto-Electronic Switch.**
Final rept.,
P. T. Ho, C. H. Lee, J. C. Stephenson, and R. R. Cavanagh. 1983, 3p
Pub. in Optics Communications 46, n3-4 p202-204, 1 Jul 83.

Keywords: *Switches, *Electrooptics, Ultraviolet radiation, Diamonds, Photoconductors, Light pulses, Reprints, Picosecond pulses, High voltage.

The authors have succeeded in using diamond as a photoconductor to switch out high voltage by picosecond ultraviolet light pulses with 80% efficiency.

*600,791*
**PB86-196292** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Technology and Economic Assessment of Optoelectronics.**
Planning rept. 23,
G. Tassey. Oct 85, 93p NBSIR-86/3369

Keywords: Electrooptics, Technology, Economic analysis, Marketing, Trends, *Foreign technology, *Optoelectronics, Research and development.

Future productivity advances in optoelectronics will come from integration of the various signal processing functions and from improved manufacturing technologies. 'Hybrid' integration, which uses oxide-based materials and integrates some of the signal processing functions, is close to commercialization. Total or 'monolithic' integration, based on gallium arsenide, may not reach commercialization for another 8-10 years. In both cases, the economic impact will be substantial. As a result, the U.S. and its major competitors, especially Japan, are making major R&D investments in optoelectronics. Worldwide R&D expenditures are expected to reach $1 billion by 1987. In terms of market penetration, fiberoptic systems will attain annual sales of more than $3 billion by 1989. The Japanese have made a national commitment to becoming the world leader in the market. Competitive positions in world markets will be determined by which countries rapidly advance all elements of the overall technological base. The base includes measurement-related methods and data which have been shown to have significant effects on productivity growth in other technological areas. Optoelectronics is projected to be equally dependent on the technology element for rapid development and market penetration.

*600,792*
**PB86-196805** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Induced Junction (Inversion Layer) Photodiode Self-Calibration.**
Final rept.,
R. L. Booker, and J. Geist. 1984, 6p
Pub. in Applied Optics 23, n12 p1940-1945 1984.

## Optoelectronic Devices & Systems

Keywords: *Photodiodes, Calibrating, Standards, Reprints.

The potential of a newly available oxide-n+-p inversion layer silicon photodiode as a radiometric standard is discussed. Data are presented relating the QE of these diodes as a function of oxide and reverse bias. The theory of a simple absolute reflectometer/detector device is described and reflectance corrections for one of the diodes is determined to establish its absolute response. Radiant power measured with this diode, at 10 wavelengths between 295 and 1014 nm, was then compared with that measured by reference to electrical substitution radiometry.

*600,793*
**PB87-104949** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Low-Cost LCD Video Display for Optical Processing.**
Final rept.,
M. Young. 1 Apr 86, 3p
Pub. in Applied Optics 25, n7 p1024-1026, 1 Apr 86.

Keywords: *Holography, Holograms, Pattern recognition, Reprints, *Liquid crystal displays, Image processing.

The paper shows that a liquid gate and a low-pass filter are needed to use a new LCD video monitor effectively in a coherent-processing system, and demonstrates the results of some simple spatial-filtering experiments.

*600,794*
**PB87-106688** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Photodiode Operating Mode Nomenclature.**
Final rept.,
J. Geist. 1986, 2p
Pub. in Applied Optics 25, n13 p2033-2034, 1 Jul 86.

Keywords: *Photodiodes, Optical measurement, Reprints.

Use of the word photoamperic is suggested as applicable to the configuration of photodiode, operational amplifier and feedback resistor that is used for high accuracy optical radiation measurements with silicon photodiodes.

## Power & Signal Transmission Devices

*600,795*
**PB86-164571** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Mode Coupling by a Longitudinal Slot for a Class of Planar Waveguiding Structures. Part 2. Applications.**
Final rept.,
P. F. Wilson, and D. C. Chang. Oct 85, 6p
See also PB86-164589.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Microwave Theory and Techniques MTT-33, n10 p988-993 Oct 85.

Keywords: *Waveguide slots, *Waveguide couplers, Trip transmission lines, Reprints, *Planar waveguides.

Coupling between two parallel-plate waveguides is investigated. Mutual excitation is due to a longitudinal slot in a common plate. The introduction of reflecting boundaries parallel to the slot allows one to model a number of planar waveguiding structures featuring a common coupling mechanism. Part II of the paper presents specific examples of the above approach along with numerical results. Examples include a rectangular coaxial transmission line, broadwall-coupled rectangular waveguides, coupled microstrips, and coupled microstrip and rectangular waveguide.

*600,796*
**PB86-164589** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Mode Coupling by a Longitudinal Slot for a Class of Planar Waveguiding Structures. Part 1. Theory.**
Final rept.,
P. F. Wilson, and D. C. Chang. Oct 85, 7p
See also PB86-164571.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Microwave Theory and Techniques MTT-33, n10 p981-987 Oct 85.

Keywords: *Waveguide slots, *Waveguide couplers, Reprints, *Planar waveguides, Integral equations, Theory.

Coupling between two parallel-plate waveguides is investigated. Mutual excitation is due to a longitudinal slot in a common plate. The introduction of reflecting boundaries parallel to the slot allows one to model a number of planar waveguiding structures featuring a common coupling mechanism. Part I of the paper details the analysis of the basic slot scattering problem based on the singular integral equation method. If one assumes that the slot is small, then closed-form algebraic model equations follow. These model equations are well-adapted to numerical parametric studies.

*600,797*
**PB86-209319** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Influence of Oxygen on the Decomposition Rate of SF6 in Corona.**
Final rept.,
M. C. Siddagangappa, R. J. Van Brunt, and A. V. Phelps. 1986, 5p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in Conference Record 1986 IEEE (Institute of Electrical and Electronics Engineers) International Symposium on Electrical Insulation, Washington, DC., June 9-11, 1986, p225-229.

Keywords: *Sulfur hexafluoride, *Electrical insulation, Decomposition, Coronas, Oxygen.

The absolute charge rates-of-production of discharge generated gaseous by-products SOF4, SOF2, SO2F2, SO2, and CO2 have been measured in compressed SF6/O2 mixtures at a constant pressure. The normalized total rate of oxyfluorides plus SO2 production per SF6 mole does not increase significantly with the addition of O2 up to 50% in SF6 and increases slowly for (O2)>50%. The formation of SO2 in all SF6/O2 mixtures was insignificant. Instead, the deposition of sulfur (S(+)ions) on the anode increased with O2 concentration. The yield of CO2 from oxidation of carbon on the electrode was also observed to increase, with O2 content. Probable mechanisms for the formation of SOF2, SO2F2, SOF4, S(+)ions, and CO2 are discussed. The measured by-product yield as a function of percent O2 are compared with the calculated maximum rate of SF6 decomposition induced by electron collision in the discharge. The theoretical model used to calculate the rate of SF6 decomposition in SF6/O2 mixtures is briefly discussed. As observed for SF6/N2 and SF6/Ne mixtures, the primary effect of O2 on SF6 decomposition appears to be retardation of the recombination of SF6 dissociation products due to dilution.

*600,798*
**PB86-246154** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Final Report: Technical Contributions to the Development of Incipient Fault Detection/Location Instrumentation,**
W. E. Anderson, J. D. Ramboz, and A. R. Ondrejka. Apr 86, 84p NBSIR-86/3392
See also PB81-188005. Sponsored by Department of Energy, Washington, DC.

Keywords: *Electrical fault location, *Power transmission lines, Instruments, Computer programs, Power lines, Electrical faults, Detection, Underground power transmission.

The transmission of electrical energy by use of underground cables is increasing. Fault location techniques have certain limitations; incipient fault detection and location would help reduce the maintenance cost of these lines as well as improve the reliability of service. The report discusses some test results related to RF-probing techniques applied to high-voltage transmission lines. The high frequency losses and attenuation in high voltage cables places certain ultimate limitations on RF-probing techniques for incipient fault detection. Time domain reflectrometry methods were employed to assess the RF-transmission properties of high voltage cables at frequencies as high as 6 GHz. Fast Fourier transform deconvolution were used to obtain loss measurements as a function of frequency. The loss mechanisms were identified. The measurement hardware and methods are discussed as well as analysis approach leading to the conclusions.

*600,799*
**PB87-106399** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Out-of-Band Response of a Coax-to-Waveguide Adapter.**
Final rept.,
D. A. Hill. 1986, 3p
Pub. in IEEE Transactions on Electromagnetic Compatibility EMC-28, n3 p156-158 Aug 86.

Keywords: *Adapters, *Waveguide couplers, Microwave equipment, Responses, Reprints.

The input impedance and transmission coefficients of a coax-to-waveguide adapter are analyzed for out-of-band frequencies. Numerical results are shown for an S-band adapter for frequencies from 2 to 10 GHz. The above-band response is frequency sensitive because of the presence of higher order propagating modes in the waveguide.

## Resistive, Capacitive, & Inductive Components

*600,800*
**AD-P002 479/4** PC **A02**/MF **A01**
National Bureau of Standards, Washington, DC.
**Excess Noise in Quartz Crystal Resonators,**
J. J. Gagnepain, M. Olivier, and F. L. Walls. 1983, 8p
Pub. in Proceedings of the Annual Symposium on Frequency Control (37th), 1-3 Jun 83, Marriott Hotel, Philadelphia, PA., AD-A136 673, p218-225.

Keywords: *Quartz resonators, *Noise(Electrical and electromagnetic), Crystal oscillators, Resonant frequency, Frequency response, White noise, Measurement, *Foreign technology, Component Reports.

Frequency and phase noise in quartz crystal resonators are studied as a function of the driving power. At low power, where the crystal behaves linearly, 1/f fluctuations of the resonance frequency are observed. At medium power the nonlinearities of the crystal significantly increase the phase fluctuations at low Fourier frequencies. At high power, thermal instabilities and chaotic behavior occur characterized by the generation of high level white noise.

*600,801*
**PATENT-4 575 690** Not available NTIS
Department of the Army, Washington, DC.
**Acceleration Insensitive Oscillator.**
Patent,
F. L. Walls, and J. R. Vig. Filed 25 Mar 85, patented 11 Mar 86, 6p PB86-182581, PAT-APPL-6-715 862 Supersedes AD-D011 621.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Crystal oscillators, *Patents, Sensitivity, Acceleration tolerance, PAT-CL-331-162.

A crystal oscillator, including two crystals of unequal acceleration sensitivity magnitude and mounted such that their respective acceleration sensitivity vectors are aligned in an anti-parallel relationship, further includes at least one electrical reactance, such as a variable capacitor, coupled to one of the crystals for providing cancellation of acceleration sensitivities. After the acceleration sensitivity vectors of the two crystals are aligned anti-parallel, the variable capacitor is adjusted until the net or resultant acceleration sensitivity vector of the pair of resonators is reduced to zero. A second electrical reactance, such as a variable capacitor, is utilized as a tuning capacitor for adjusting the oscillator's output frequency to the desired value, while maintaining the cancellation of acceleration sensitivities.

*600,802*
**PB86-193810** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

**International Comparison of Current Transformer Calibrations.**
Final rept.,
W. Schwitz, R. Kampfer, A. Braun, T. M. Souders, and W. J. M. Moore. 1985, 5p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM34, p234-238 Jun 85.

Keywords: *Current transformers, Calibrating, Reprints.

An international comparison of current transformer calibrations between five metrology laboratories has been conducted. The measurements were made at current ratios ranging from 1 A:1 A to 200 A:1 A at 10, 100, and 200 percent of rated current and from 5 A:5 A to 200 A:5 A at 1, 10, 100, and 200 percent of rated current, at a frequency of 50 Hz. Several ratios have also been compared at 60 Hz.

*600,803*
**PB86-210259** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Self-Heated Thermistor Flowmeter for Flow Measurement in a Thermosyphon Solar Hot Water System.**
Final rept.,
A. H. Fanney, and B. P. Dougherty. 1986, 14p
Pub. in Proceedings of ASME (American Society of Mechanical Engineers) Solar Energy Conference (SED 8th Annual), Anaheim, CA., April 13-16, 1986, p1-10.

Keywords: *Thermistors, Flowmeters, Flow measurement, Calibrating, Dissipation factor, *Solar waterheaters, Thermosyphons.

The development and calibration of a self-heated thermistor anemometer is described. The variation in thermistor power dissipation as a function of fluid temperature and velocity is presented. A thermal analysis of the glass-encapsulated thermistor bead is described which leads to an experimental technique for determining the effective radius and thermal conductivity of the thermistor probe. A dimensionless heat transfer analysis is performed and the results compared to empirical correlations. The thermistor flowmeter, which evolves from the investigation, is used to measure the buoyancy-induced flow in a thermosyphon solar hot water system.

*600,804*
**PB86-214228** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.
**Fourier Analysis of Impedance Spectra for Electroded Solid Electrolytes.**
Final rept.,
A. D. Franklin, and H. J. deBruin. 1983, 10p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Physica Status Solidi A-Applied Research 75, n2 p647-656 1983.

Keywords: *Solid electrolytes, *Electrolytic cells, Fourier analysis, Impedance, Spectra, Electrical properties, Frequency response, Reprints.

The electrical properties of a solid conductor with its attached electrodes can often be represented by an equivalent circuit involving only a few parameters. The cell's frequency response, which is imposed by its materials' behavior, can then be expressed in terms of these circuit parameters. Critical elements in the logical chain then are the degree of fit of the equivalent circuit to the data, and the relationship of the circuit parameters to the material properties. The paper will be concerned with the first of these critical elements, the fitting of the circuit to the data.

*600,805*
**PB86-231446** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Measurements of the Electromagnetic Shielding Capabilities of Materials.**
Final rept.,
P. F. Wilson, J. W. Adams, and M. T. Ma. 1986, 4p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Special Issue on Radio Measurement Methods and Standards 74, n1 p112-115 Jan 86.

Keywords: *Electromagnetic shielding, Measurement.

Electromagnetic shielding is typically measured in terms of insertion loss, that is, the reduction in the fields coupled between a transmitter and a receiver which results from interposing the shield material. Although the insertion loss concept is simply stated, questions arise when one attempts to interpret specific insertion loss measurements. Insertion loss data depend not only on the inherent shielding effectiveness of the material, but also on the antenna types used for the measurement, the incident field distribution, the sample size, a possible contact impedance between the test material and its mount, and other factors. For a given sample of shield material, varying these factors can lead to a large range of possible measured insertion loss values. Both the above considerations and existing shielding effectiveness measurement systems will be discussed briefly in the paper. The emphasis will be on the potential difficulties in making even relative comparisons of results and on the importance of understanding how the measurement system used affects data.

*600,806*
**PB86-240744** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Ultrasonic Transducers.**
Final rept.,
W. Sachse, and N. Hsu. 1986, 7p
Pub. in Encyclopedia of Materials Science and Engineering, v7 p5192-5198 1986.

Keywords: *Transducers, Ultrasonic frequencies, Reprints.

No abstract available.

*600,807*
**PB86-244183** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Center for Electronics and Electrical Engineering.
**Study of Techniques for Measuring the Electromagnetic Shielding Effectiveness of Materials.**
Technical note,
P. F. Wilson, and M. T. Ma. May 86, 72p NBS/TN-1095
Also available from Supt. of Docs as SN003-003-02735-9 Sponsored by Army Aviation Systems Command, St. Louis, MO.

Keywords: *Electromagnetic shielding, Measurement, Shielding, Mathematical models.

The report covers a number of measurement approaches which are studied, including the use of a shielded room, coaxial transmission line holders, time domain signals, the dual TEM cell, and an apertured TEM cell in a reverberation chamber. In each case the system's frequency range, test sample requirements, test field type, dynamic range, time required, analytical background, and present data taken on a common set of materials are considered.

*600,808*
**PB87-110078** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Discussion on 81 SM 322-7 'Breakdown of Rod-Plane Gaps in SF6 under Positive Switching Impulses' by H. Aris and K. D. Srivastava.**
Final rept.,
R. J. Van Brunt. Mar 82, 1p
Pub. in Institute of Electrical and Electronics Engineers Transactions on Power Apparatus and Systems PAS-101, n3 p546 Mar 82.

Keywords: *Sulfur hexafluoride, Dielectric breakdown, Electric insulation, Surges.

No abstract available.

*600,809*
**PB87-114914** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Use of Deconvolution Methods in Characterizing Electrical Sensors.**
Final rept.,
R. H. McKnight, C. Fenimore, and J. Lagnese. 1986, 3p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Institute of Electrical and Electronics Engineers Pulsed Power Conference (5th), Arlington, VA., June 10-12, 1985, p176-178 1986.

Keywords: *Detectors, *Electronic engineering, *Voltage dividers, Resistors, Capacitors, Measurement.

Deconvolution methods have been applied to measurements made with different electrical sensors including resistive and capacitive dividers. Deconvolved and directly measured waveforms have been compared with good results.

*600,810*
**PB87-115416** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Onset of Chaos in the rf-Biased Josephson Junction.**
Final rept.,
R. L. Kautz, and J. C. Macfarlane. 1986, 12p
Pub. in Physical Review A 33, n1 p498-509 Jan 86.

Keywords: *Josephson junctions, Superconductivity, Reprints, Chaos, Melnikov method.

The onset of chaos in the rf-biased Josephson junction is studied through numerical simulations. It is shown that the chaotic region predicted by the method of Melnikov spans only a narrow region of rf amplitudes and consists of weakly chaotic solutions which maintain phase lock with the rf bias. The experimentally observed threshold of chaos is shown to coincide with the onset of unlocked chaotic behavior at higher rf amplitudes.

*600,811*
**PB87-132734** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Irradiation Effects on Organic Insulators.**
Progress rept. 1 Oct 84-1 Oct 85,
M. B. Kasen. 1986, 8p
Contract DE-AC01-84ER52112
Sponsored by Department of Energy, Washington, DC. Div. of Magnetic Fusion Energy.
Pub. in Annual Progress Report on Special Purpose Material for Magnetically Confined Fusion Reactors (8th), DOE/ER-0113/5 p25-32 1986.

Keywords: *Electrical insulation, Cable insulation, Superconducting magnets, Cryogenics, Neutron irradiation, Torsion, Shear strength, Fracture properties, *Physical radiation effects, Fusion reactors.

Progress in development of specimens and test methods required for studies of the significant parameters influencing mechanical property degradation of organic insulators under combined cryogenic temperature and neutron irradiation is reported. Standard specimens in rod form, 3.2 mm diameter in both neat resin form and as uniaxially reinforced composites have been produced in several epoxy systems and in one bismaleimide polyimide system. Test methods permitting assessment of irradiation influence by torsional testing have been developed. A method for determining the influence on fracture energy has also been developed.

## Semiconductor Devices

*600,812*
**PB86-164480** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**High-Accuracy Physical Modeling of Submicrometer MOSFETs.**
Final rept.,
C. L. Wilson, P. Roitman, and J. L. Blue. 1985, 13p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices ED-32, n7 p1246-1258 Jul 85.

Keywords: *Metal oxide transistors, *Field effect transistors, *Mathematical models, Finite element analysis, Simulation, Reprints, *MOSFET.

When short-channel MOSFET transistor models are compared to experimental data, the uncertainty in some of the physical input variables often requires that some of the input variables be adjusted to fit the data. This uncertainty is increased by a lack of knowledge of process sensitivity information on critical parameters. These uncertainties have been eliminated using a two-dimensional finite-element model of a MOSFET with no free parameters. The model is compared to four self-aligned silicon-gate n-channel MOSFET's with channel lengths of 0.80, 1.83, 2.19, and 8.17 microme-

ters. The 0.80, 1.83, and 8.17 micrometer devices have phosphorus sources and drains. The 2.19-micrometer device has an arsenic source and drain. Using the data obtained from the measurements described in the work, it is possible to model the drain current for all of the transistors studied without adjustable parameters. If sufficiently accurate parameters are available, these methods allow the characteristics of submicrometer transistors to be predicted with + or - 5-percent accuracy. These simulations show that the observed short-channel effects can be accounted for by existing mobility data and a simple empirical model of these data.

*600,813*
**PB86-182482** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Release Notes for STAT2 Version 2.00A: An Addendum to NBS Special Publication 400-75. Documentation,**
C. H. Ellenwood, and R. L. Mattis. Jan 86, 19p
NBSIR-85/3292A, NBS/SW/DK-86/005A
For system on diskette, see PB86-182490.

Keywords: *Wafers, *Computer programs, Statistical analysis, Semiconductor devices, Test equipment, Data processing, Map.

STAT2 is a FORTRAN program which is used to analyze and display data from microelectronic test structures fabricated on semiconductor wafers. The program reads data as a two-dimensional array, extracts sample statistical values, identifies outliers, calculates replacement values for outliers, and makes histograms and circular gray-tone data maps. Version 2.00A is an adaptation of STAT2 to run under Version 3.2 of the RSX-11M operating system. The operating system is used on the automatic tester which acquires the test structure data. Data can then be taken and analyzed on the same system.

*600,814*
**PB86-182490** CP **T99**
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Release Notes for STAT2 Version 2.00A: An Addendum to NBS Special Publication 400-75 (for Microcomputers).**
Software,
R. L. Mattis, and C. H. Ellenwood. Jan 86, 2 diskettes NBSIR-85/3292, NBS/SW/DK-86/005
See also PB84-127455.
The software is contained on 8 1/4-inch diskette, single sided, double density, compatible with the DEC LSI-11/23 microcomputer. Diskettes are in thr ASCII format. Call NTIS Computer Products for price. Price includes documentation, PB86-182482.

Keywords: *Software, Integrated circuits, Statistical analysis, Tests, Wafers, STAT2 computer program.

STAT2 is a FORTRAN program which is used to analyze and display data from microelectronic test structures fabricated on semiconductor wafers. The program reads data as a two-dimensional array, extracts sample statistical values, identifies outliers, calculates replacement values for outliers, and makes histograms and circular gray-tone data maps. Version 2.00A is an adaptation of STAT2 to run under Version 3.2 of the RSX-11M operating system. The operating system is used on the automatic tester which acquires the test structure data. Data can therefore be taken and analyzed on the same system...Software Description: The Software is written in the FORTRAN programming language for implementation on a DEC LSI - 11/23 microcomputer using the RSX - 11M/3.2 operating system. Memory requirement is 30K.

*600,815*
**PB86-188489** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Comparison of Microelectronic Test Structures for Propagation Delay Measurements.**
Final rept.,
D. J. Radack, C. T. Yao, L. W. Linholm, K. F. Galloway, and H. C. Lin. 1985, 8p
Pub. in Microelectronics Jnl. 16, n6 p39-46 1985.

Keywords: *Integrated circuits, Test equipment, Propagation, Inverters, Reprints, *Very large scale integration, Delay, CMOS.

Propagation delay is a parameter which needs to be accurately measured for characterization of VLSI fabrication technologies and VLSI circuit design. In the experiment, three different microelectronic test structures or test circuits were used to measure the propagation delay of a minimally sized CMOS inverter. The measured results and a comparison of the test circuits are presented.

*600,816*
**PB86-193851** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Focused-Beam vs. Conventional Bright-Field Scanning Microscopy for Integrated Circuit Metrology.**
Final rept.,
D. Nyyssonen. 1985, 6p
Pub. in SPIE Micron and Submicron Integrated Circuit Metrology 565, p102-107 1985.

Keywords: *Integrated circuits, *Dimensional measurement, Metrology, Microscopy, Line width, Reprints.

Current optical instrumentation being developed for critical dimension measurements in the integrated circuit industry is following one of two very different optical designs, i.e., either a focused laser beam which scans the wafer or the more conventional bright-field microscope. Traditional optical design lore has described these systems as 'equivalent' based on the principle of reciprocity. More recent research has shown that the responses of these two types of systems are not equivalent for imaging of structures patterned in thin films such as those found in integrated circuit wafer fabrication. This lack of reciprocity is the result of the dependence of the diffraction pattern on the angle of incidence of the illumination. The impact of the lack of reciprocity on the design and calibration of critical dimension measurement systems is discussed.

*600,817*
**PB86-202561** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**VLSI Package Reliability Workshop Report.**
Final rept.,
D. D. Zimmerman, and H. A. Schafft. 1983, 4p
Pub. in Proceedings of the Annual Symposium on Reliability Physics (21st), Phoenix, AZ., April 5-7, 1983, p320-323.

Keywords: *Integrated circuits, *Electronic packaging, Reliability, Semiconductor devices, Materials, Moisture, Packaging, Very large scale integration.

The report summarizes remarks made by six panelists in an evening workshop meeting held as part of the 1983 International Reliability Physics Symposium. The panelists provided an overview of package design and measurement considerations that arise because of special requirements of packaging VLSI semiconductor chips. Considerations in the following areas were discussed: package materials, design, and construction; thermal management and characterization; and moisture and hermeticity measurements.

*600,818*
**PB86-214723** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Center for Electronics and Electrical Engineering.
**Model for the Charge-Pumping Current Based on Small Rectangular Voltage Pulses.**
Final rept.,
R. A. Wachnik, and J. R. Lowney. 1986, 14p
Pub. in Solid State Electronics 29, n4 p447-460 1986.

Keywords: *Metal oxide transistors, *Field effect transistors, Models, Bandwidth, Reprints, *MOSFET, Charge pumping, Current leakage, Voltage pulses.

The charge-pumping current results from recombination associated with the silicon oxide interface traps under the gate of a MOSFET when a voltage pulse is applied to the gate. A model is proposed which predicts this current as a function of the frequency, amplitude, and average voltage of pulses with peak-to-peak amplitudes less than the difference between the flat-band and inversion voltages and with pulse transitions fast enough so that negligible capture or emission occurs during the transition. The model is based on Shockley-Read-Hall traps segregated by energy and capture cross section into traps which capture only and traps which tend to emit before capture. It predicts the dominant behavior of the measured current and with the inclusion of surface potential fluctuations and a distribution of cross sections it agrees well with experiment.

*600,819*
**PB86-231107** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Accurate Current Calculation in Two-Dimensional MOSFET Models.**
Final rept.,
C. L. Wilson, and J. L. Blue. 1985, 9p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices ED-32, n10 p2060-2068 Oct 85.

Keywords: *Metal oxide transistors, *Mathematical models, *Electric current, Finite element analysis, Partial differential equations, Integrated circuits, Simulation, Reprints, *MOSFET, Very large scale integration, Two dimensional.

Two-dimensional simulations of MOSFET's are widely used for the design of short-channel transistors used in VLSI circuits. These models use low order methods of discretization of solution variables. In the paper, a method of current calculation is presented which works with these methods and yields good accuracy. The method uses integration of the solution variables, rather than differentiation, and is similar to applying Ohm's law in two dimensions.

*600,820*
**PB86-231115** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Boron Diffusion In Silicon.**
Final rept.,
J. F. Marchiando, P. Roitman, and J. Albers. 1985, 9p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices ED-32, n11 p2322-2330 Nov 85.

Keywords: *Silicon, *Boron, Metal oxide transistors, Diffusion, Reprints, *Ion implantation, MOSFET, Two dimensional.

Well-defined control of high- and low-temperature anneals of boron implanted in silicon is important in the calculation of shallow p-n junction profiles used in MOSFET's. Here, a sample matrix of boron implanted into silicon over a range of fluences and annealing temperatures is considered. The matrix of samples was measured by SIMS (secondary ion mass spectrometry). The measured profiles were compared with simulations from an annealing/diffusion model. Calculations of the annealed profiles were found to be in agreement with the SIMS data at temperatures greater than 1000 C. At lower temperatures, the profiles exhibit effects due to implantation damage which are not included in the diffusion model.

*600,821*
**PB86-239266** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Modeling GaAs/AlGaAs Devices: A Critical Review.**
Final rept.,
H. S. Bennett. Jan 85, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Circuits Devices Magazine 1, n1 p35-42 Jan 85.

Keywords: *Transistors, *Gallium arsenides, Semiconductor devices, Monte Carlo method, Reprints, Aluminum gallium arsenides.

Device models for GaAs devices and GaAs/AlGaAs heterostructures are much less advanced than those for silicon devices. The paper critically reviews recent advances in the modeling of GaAs/AlGaAs devices. It is based on the examination of five selected device models which contain features common to the majority of device models for heterostructure bipolar and field effect transistors. Areas requiring improved measurement techniques on processed GaAs and improved physical concepts for GaAs/AlGaAs device models are identified.

*600,822*
**PB86-239274** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.

**Improved Physics for Simulating Sub-Micron Bipolar-Devices.**
Final rept.,
H. S. Bennett, and D. E. Fuoss. 1985, 7p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices 32, n10 p2069-2075 1985.

Keywords: *Field effect transistors, Semiconductor doping, Mathematical models, Reprints.

The conventional device physics in most numerical simulations of bipolar transistors may not predict correctly the measured electrical performance of shallow, heavily doped emitters and bases. The paper presents improved device physics for numerical simulations of solid-state devices with densities up to about 3 x 10 to the 20th power/cucm and with junction depths as small as 0.1 micrometers. This improved device physics pertains to bandgap narrowing, effective intrinsic carrier concentrations, carrier mobilities, and lifetimes. When this improved device physics is incorporated into device analysis codes such as SEDAN and then used to compute the electrical performance of npn transistors, the predicted values agree very well with the measured values of the current-voltage characteristics and dc common emitter gains for junction depths between 10 micrometers and 0.16 micrometers.

*600,823*
**PB87-119590** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Simple Model for Separating Interface and Oxide Charge Effects in MOS Device Characteristics.**
Final rept.,
K. F. Galloway, M. Gaitan, and T. J. Russell. 1984, 5p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science NS-31, n6 p1497-1501 Dec 84.

Keywords: *Interfaces, *Metal oxide transistors, *Radiation effects, *Field effect transistors, Traps, Density(Mass/volume), Reprints.

A simple model to describe radiation effects on MOSFET electrical characteristics is presented. The key assumption is that mobility degradation in an enhancement mode MOSFET is predominantly due to charged interface traps. Model predictions are compared with measured values of interface trap density and device I-V curves.

*600,824*
**PB87-119608** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Measurement of Radiation-Induced Interface Traps Using MOSFETs.**
Final rept.,
M. Gaitan, and T. J. Russell. 1984, 5p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science NS-31, n6 p1256-1260 Dec 84.

Keywords: *Radiation effects, *Traps, *Interfaces, *Measurement, Gamma irradiation, Irradiation, Silicon, Silicon oxides, Density(Mass/volume), Metal oxide transistors, Field effect transistors, Reprints.

The effect of gamma irradiation on the density of SiO2/Si interface traps was measured using n- and p-channel MOSFETs. The density of traps was measured by a charge pumping measurement method and by a technique based on the slope of the transistor ln (Id)-Vg characteristics in weak inversion. An increase in the density of interface traps with dose is observed with a greater increase just above compared to just below the center of the silicon bandgap.

*600,825*
**PB87-122404** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**ASTM (American Society of Testing and Materials) Standard Test Methods for the Semiconductor Industry.**
Final rept.,
R. I. Scace. 1980, 8p
Pub. in Proceedings of Semicon/Europa 1980 Technical Symposium, Zurich, Switzerland, March 13, 1980, p202-209.

Keywords: *Standards, *Semiconductor industry, *Test methods, International cooperation.

The unique characteristics of the U.S. voluntary standards system, as distinct from the standards systems of most other countries, are described. The roles of JEDEC, ISHM, SAE, and the MIL standards system are briefly reviewed. The work of ASTM Committee F-1 over the past 24 years in developing standards for the semiconductor industry is described in detail. The process of standards development is described, and the value of inter-laboratory tests in evaluating the precision and accuracy of test methods is pointed out. The close relationship which has been maintained with both DIN Normenausschuss Materialprufung 221 and the Semiconductor Equipment and Materials Institute standards committee is described in detail. An appendix contains listings of the ASTM standards for semiconductor applications, classified by topic.

*600,826*
**PB87-122693** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Electron Detection Modes and Their Relation to Linewidth Measurement in the Scanning Electron Microscope.**
Final rept.,
M. T. Postek. 1986, 4p
Pub. in Proceedings of the Annual Meeting of the Electron Microscopy Society of America (44th), Albuquerque, NM., August 10-15, 1986, p646-649.

Keywords: *Backscattering, *Electron microscopy, *Electron microscopy, *Semiconductors, Line width, Electron beams, Scanning, Research projects, Measurement, *Electron detection.

The basic premise underlying the use of the scanning electron microscope for linewidth measurement for semiconductor research and production applications is that the video image acquired, displayed, and ultimately measured reflects accurately the structure of interest. The paper demonstrates that depending upon the mode of electron detection (secondary, backscattered, or converted backscattered secondary electrons) and accelerating voltage used to image and measure the structure of interest, a variety of results can be obtained. The reasons for these differences are discussed relative to the coupling of the type of work with electron beam/sample interaction modeling to enable the acquisition of more precise linewidth measurements.

*600,827*
**PB87-122701** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Wafer Mapping of Electrically Active Defects.**
Final rept.,
R. Y. Koyama. 1978, 9p
Sponsored by Department of Energy, Washington, DC., and Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Proceedings of ECS Topical Conference on Characterization Techniques for Semiconductor Materials and Science, Seattle, WA., May 21-24, 1978, p220-228.

Keywords: *Wafers, Mapping, Defects, Semiconductor devices, Measurement.

Although deep level measurements on packaged devices are common practice, these measurements cannot generally be made at the wafer level because the required apparatus has not been available. However, such wafer level measurements would provide to the process engineer a valuable analytical tool for process control or process diagnostics. Appropriate apparatus to allow deep level measurements on processed wafers has been designed and constructed. Its use is illustrated by the measurement of wafer maps showing the variation of electrically active defect density across a wafer and the correlation of defect density with device electrical characteristics.

*600,828*
**PB87-122719** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Techniques for Characterizing Defects in Starting Silicon Wafers Using TSM (Thermally Stimulated Current and Capacitance Measurements).**
Final rept.,
R. Y. Koyama. 1978, 8p
Sponsored by Department of Energy, Washington, DC., and Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Proceedings of ECS Topical Conference on Characterization Techniques for Semiconductor Materials and Science, Seattle, WA., May 21-24, 1978, p53-60.

Keywords: *Silicon, *Metal oxide transistors, Waters, Capacitance, Semiconductors, *Defects(Materials), Low temperature research, Silicon dioxide, Vapor deposition, Measurements, *Metal oxide semiconductors, *Defects(Materials).

Since thermally stimulated current and capacitance measurements (TSM) can utilize a metal-oxide-semiconductor (MOS) capacitor as the test vehicle for defect characterization, an MOS capacitor fabricated with relatively low temperature processes should be useful for studying defects in starting material. Several processes were investigated. The process which yielded the most consistent devices utilized chemical vapor deposition (CVD) of silicon dioxide at 400C along with a 400C microalloy treatment. Thermally stimulated current measurements on MOS capacitors fabricated in this way were successful in detecting gold which was purposely introduced into a starting wafer.

*600,829*
**PB87-122743** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Use of Acoustic Emission as a Test Method for Electronic Interconnections and Joints.**
Final rept.,
G. G. Harman. 1981, 7p
Pub. in Proceedings of International Conference on Soft Soldering in Electronics and Precision Mechanics, Munich, Germany, November 11-12, 1981, p104-110.

Keywords: *Welded joints, *Acoustic detectors, *Microelectronics, *Circuit interconnections, Joints(Junctions), Monitors, Nondestructive tests, Stresses, Surface waves, Sensitivity, *Acoustic emissions.

The use of acoustic emission (AE) to determine the integrity of various microelectronic joints is relatively new. Considerable success has been achieved using AE as an in-process production monitor, and some of these uses are reviewed. However, implementation problems have been experienced using AE as an after-production screen. These problems result from the small size of the electronic components as well as the difficulty of applying an appropriate nondestructive mechanical or thermal stress to the tiny joints. The small size also causes difficulty in interpreting the AE signals. These and other problems are discussed and various solutions proposed. The paper describes a newly designed miniature AE detector in a TO-5 sized package appropriate for microelectronic use that has high sensitivity to surface waves and contains its own built-in 40-dB preamplifier.

*600,830*
**PB87-127957** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Use of Charge Pumping to Characterize Generation by Interface Traps.**
Final rept.,
R. A. Wachnik. 1986, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices ED-33, n7 p1054-1061 Jul 86.

Keywords: Semiconductor diodes, Electric current, Silicon, Silicon dioxide, Interfaces, Field effect transistors, Reprints, *Charge pumping, MOSFET.

A small rectangular pulse technique for measuring charge-pumping current has been proposed as a method to characterize interface traps near midgap. It is shown theoretically and experimentally that the small rectangular pulse technique can be used to predict the surface generation current measured on a MOSFET or a gated diode. The new technique has the advantage that the measured current is at least 10 to 100 times larger than the surface generation current.

*600,831*
**PB87-131488** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

**Modeling MOS Capacitors to Extract Si-SiO2 Interface Trap Densities in the Presence of Arbitrary Doping Profiles.**
Final rept.,
H. S. Bennett, M. Gaitan, P. Roitman, T. J. Russell, and J. S. Suehle. 1986, 7p
Sponsored by Defense Nuclear Agency, Washington, DC.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices ED 33, n6 p759-765 Jun 86.

Keywords: *Electron traps, *Hole traps, *Capacitors, *Interfaces, Gamma rays, Semiconductor doping, Silicon dioxide, Silicon, Reprints, Metal oxide semiconductors.

A conventional Poisson solver has been used to calculate the quasi-static capacitance of an MOS capacitor. The effects of an energy dependent Si-SiO2 interface trap density and of an arbitrary silicon substrate doping profile have been included. The model has been used to calculate the quasi-static C-V characteristics and to compare them with those measured using Kuhn's technique for as-received and for gamma-irradiated p-type and n-type silicon MOS capacitors. The substrate doping profiles were obtained from high-frequency C-V curves. Experimental and theoretical C-V curves were made to agree by varying the voltage offset due to fixed oxide charge and both the magnitude and the energy distribution of interface trapped charge.

*600,832*
**PB87-134896** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Performance Trade-Off for the Insulated Gate Bipolar Transistor: Buffer Layer Versus Base Lifetime Reduction.**
Final rept.,
A. R. Hefner, and D. L. Blackburn. 1986, 12p
Pub. in Proceedings of Annual IEEE (Institute of Electrical and Electronics Engineers) Power Electronics Specialists Conference (17th), Vancouver, Canada, June 23-27, 1986, p27-38.

Keywords: *Transistors, Mathematical models, *Bipolar transistors, Power transistors, One dimensional, Transients.

A one-dimensional analytic model for the Insulated Gate Bipolar Transistor (IGBT) which includes a high-doped buffer layer in the low-doped bipolar transistor base is developed. The model is used to perform a theoretical trade-off study between IGBTs with and without the buffer layer. The study is performed for devices of equal breakdown voltages, and the critical parameters chosen to 'trade-off' are turn-off switching energy loss (related to turn-off time) and on-state voltage, both at a given current. In the study, as in reality, the two critical parameters are varied by: (1) adjusting the doping concentration and thickness of a buffer layer included as part of the bipolar transistor base, (2) adjusting the lifetime in the lowly doped bipolar transistor base with no buffer layer included, or by (3) a combination of (1) and (2). The results of the model predict that for equal breakdown voltages, an optimized device with a buffer layer has less switching energy loss for a given on-state voltage than an optimized device with no buffer layer.

*600,833*
**PB87-134904** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Power MOSFET Failure during Turn-Off: The Effect of Forward Biasing the Drain-Source Diode.**
Final rept.,
D. W. Berning, and D. L. Blackburn. 1986, 5p
Pub. in Proceedings of Conference on Record 1986 IEEE (Institute of Electrical and Electronics Engineers) Industry Applications Society Annual Meeting, Denver, CO., September 28-October 3, 1986, p335-339.

Keywords: *Metal oxide transistors, *Field effect transistors, Nondestructive tests, Failure, Reliability(Electronics), *MOSFET, Second breakdown, Power transistors.

The effects on the turn-off failure of power MOSFETs which result from forward biasing the intrinsic drain-source diode immediately prior to turn-off are discussed. A nondestructive test circuit is used to measure the turn-off characteristics of individual devices under a variety of conditions. It is shown that the drain voltage at which the device fails decreases as either the diode forward current or the reverse recovery current is increased. If the diode is forward biased, the voltage at failure can be less than one-half of the voltage at which the device fails if the diode has not been forward biased (and often less than one-half the manufacturer-rated voltage capability for the device). Also, if turn-off of the MOSFET is attempted with the diode conducting, the device loses its fast turn-off capability due to charge storage effects. A parallel resonant power converter circuit is employed to demonstrate how the intrinsic drain-source diode may and may not be used safely in practical applications.

*600,834*
**PB87-140307** PC **A03**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Cobalt-60 Facilities Available for Hardness Assurance Testing.**
Final rept.,
J. C. Humphrey, and C. M. Dozier. Nov 86, 31p NBSIR-86/3480
Sponsored by Defense Nuclear Agency, Washington, DC.

Keywords: *Microelectronics, *Test facilities, Cobalt 60, Gamma rays, *Irradiation devices, *Radiation hardening, *Gamma sources.

The report contains a list of cobalt-60 gamma-ray irradiation facilities that are available for hardness assurance testing of electronic devices. A summary of source type, absorbed-dose rates, experimental volume available, and other pertinent information is given for each facility.

## General

*600,835*
**PB86-160967** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Near-Zero Bias Arrays of Josephson Tunnel Junctions Providing Standard Voltages up to 1 V.**
Final rept.,
J. Niemeyer, J. H. Hinken, and R. L. Kautz. Jun 85, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-34, n2 p185-187 Jun 85.

Keywords: *Josephson junctions, Integrated circuits, Superconductivity, Microwave equipment, Reprints, *Voltage standards.

Josephson voltage standards use microwave-induced constant voltage steps occurring due to the ac Josephson effect. Existing standards can be considerably simplified and their accuracy improved by using a large number of series-connected Josephson tunnel junctions which are operated in the zero current step mode. For this purpose superconducting millimeter wave integrated circuits have been designed, fabricated, and tested. The circuits consist of a broadband taper between the rectangular waveguide and the planar structure, the Josephson junction series, a well-matched load, and dc pads. Circuits with various numbers of junctions have been fabricated by photo-lithographic techniques and tested at 4.2 K in liquid helium. The version with 1474 junctions produced voltages up to 1.2 V when operated at 90 GHz.

*600,836*
**PB86-163607** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Calibration of Standard Wattmeters Using a Capacitance Bridge and a Digital Generator.**
Final rept.,
N. M. Oldham, and O. Petersons. Dec 85, 4p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-34, n4 p521-524 Dec 85.

Keywords: *Wattmeters, *Capacitance bridges, *Calibrating, Digital systems, Signal generators, Reprints, Comparators.

A method for calibrating high-accuracy wattmeters is described. The technique is a modification of a previously described approach that utilizes a power bridge based on a current comparator. In such a bridge the test current of the wattmeter is balanced with a known current that is proportional to the test voltage. The measurement circuit described employs a high-voltage capacitance bridge in place of a special current comparator that was used in the previous system. High sensitivity and large ratios of the capacitance bridge enable using high impedances, such as stable gas-dielectric capacitors and resistors having low-power dissipation for the generation of reference currents. The voltage on the standard impedances is adjusted with inductive dividers to obtain any power factor between zero and one, lead and lag. A digitally synthesized dual-channel signal source serves as a stable source of voltage and current, and thus of 'phantom' power.

*600,837*
**PB86-164472** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Shielding-Effectiveness Measurements with a Dual TEM (Transverse Electromagnetic) Cell.**
Final rept.,
P. F. Wilson, and M. T. Ma. Aug 85, 6p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electromagnetic Compatibility EMC-27, n3 p137-142 Aug 85.

Keywords: *Electromagnetic shielding, Measurement, Reprints, *Transverse electromagnetic cells.

Small-aperture theory is used to investigate the dual transverse electromagnetic (TEM) cell. Analyzing coupling through an empty versus loaded aperture leads to a simple model of dual-TEM-cell material shielding-effectiveness (SE) measurements. Experimental data are compared to theory with good agreement in the case of an empty aperture. Some of the difficulties in analyzing a loaded aperture are discussed.

*600,838*
**PB86-164563** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Dual-Channel Automated Comparator for AC-DC Difference Measurements.**
Final rept.,
E. S. Williams, and J. R. Kinard. Jun 85, 5p
Sponsored by Department of Defense, Washington, DC.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-34, n2 p290-294 Jun 85.

Keywords: *Comparators, *Calibrating, Electrical measuring instruments, Reprints.

An automated ac-dc difference calibration system is described. The system incorporates a new electronic comparator which determines ac-dc differences of thermal voltage converters (TVC's) by simultaneously measuring the difference between nearly equal ac and dc voltages with both the test and standard instruments. The comparator consists essentially of two practically identical channels each containing a digital-to-analog converter balancing circuit, an operational amplifier to amplify voltage imbalance, and an integrator circuit in which a capacitor is charged during an accurately controlled 10-s period. The difference between the ac and dc voltages applied to the test and standard TVC's is computed from differences in capacitor voltages, and the ac-dc difference is derived from the variation between the test and standard channel indications of the voltage difference. Measurements are made in about half the time required for our manual procedures.

*600,839*
**PB86-166618** PC **A08**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**U.S. Access to Japanese Technical Literature: Electronics and Electrical Engineering. Proceedings of a Seminar Held at Gaithersburg, Maryland on June 24-25, 1985. Volume 1. Selected Presentations.**
Final rept.,
E. L. Brady. Jan 86, 151p NBS/SP-710
Also available from Supt. of Docs as SN003-003-02709-0. Library of Congress catalog card no. 85-600637. Sponsored by Institute of Electrical and Electronics Engineers, Inc., New York.

Keywords: *Technical reports, *Electrical engineering, *Electronic engineering, Availability, Japan.

On June 24-25, 1985, NBS and IEEE cosponsored a seminar at NBS to examine the need for improved access to Japanese technical information and to explore possible approaches to satisfy those needs. To limit the discussion to practical dimensions, the technical subject matter was restricted to electrical and electronics engineering. The program was designed to provide an opportunity for individuals representing Congress, the practicing engineering community, industry, and the educational community to voice their concerns and their needs.

*600,840*
**PB86-191814** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Research for Electric Energy Systems - An Annual Report (1985),**
R. E. Hebner. Mar 86, 88p NBSIR-86/3316
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.

Keywords: *Electric power, Electric measuring instruments, Dielectrics, Dielectric breakdown, Sulfur hexafluoride, Electrical insulation, Interfaces, Space charge, Insulating oil, Electric fields, Magnetic fields.

The report documents the technical progress in the five investigations which make up the project 'Support of Research Projects for Electrical Energy Systems,' Department of Energy Task Order Number 137, funded by the U.S. Department of Energy's Office of Energy Systems Research and performed in the Electrosystems Division of the U.S. National Bureau of Standards.

*600,841*
**PB86-193802** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Length and Mass Div.
**Automatic High-Precision Audiofrequency Capacitance Bridge.**
Final rept.,
R. D. Cutkosky. 1985, 7p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-34, n3 p383-389 Sep 85.

Keywords: *Capacitance bridges, Audio frequencies, Reprints.

A compact transformer-ratio-arm bridge has been built in which the balance point is automatically determined with the aid of an internal microprocessor. The instrument described in the paper can operate from 20 Hz to 20 kHz, and has three ranges; 12, 120, and 1200 pF. The instrument can resolve one part in 10 to the 8th power of full scale above 400 Hz, and can be fully controlled over its IEEE-488 bus interface.

*600,842*
**PB86-195757** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Precision Phase Angle Calibration Standard for Frequencies up to 50 kHz.**
Final rept.,
R. S. Turgel. Dec 85, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-34, n4 p509-516 Dec 85.

Keywords: *Standards, *Calibrating, *Frequency measurement, Waveforms, Radiofrequency generators, Phase angle, Phase meters, Reprints.

A Phase Angle Calibration Standard covering a frequency range from 2 Hz to 50 kHz has been designed and constructed. Digital waveform generation is used to provide sinusoidal analog outputs having precisely settable phase angles. Output voltages are independently adjustable from 0.5 to 100 V rms on both channels. An auto-zero feed back loop compensates for differential phase errors of the output amplifiers.

*600,843*
**PB86-201811** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Ellipsometric Metrology of Ultrathin Films: Dual Angle of Incidence.**
Final rept.,
D. Chandler-Horowitz. 1985, 5p
Pub. in Proceedings of the SPIE (Society for Photo-Optical Instrumentation Engineers) International Conference on Micron and Submicron Integrated Circuit Metrology, San Diego, CA., August 22-23, 1985, v565 p93-97.

Keywords: *Thin films, *Metrology, Measurement, Incidence, Error analysis, Substrates, Silicon, Ellipsometric metrology, Ultrathin films.

Single angle of incidence ellipsometric measurements have been extended to dual angle measurements on our newly constructed multi-method precision ellipsometer in order to better determine the optical constants of a substrate. Following the measurement error analysis that was prescribed in an earlier paper for single angle of incidence and fixed wavelength measurements, the results for dual angle of incidence are presented here. Using an Explicit Error Analysis (EEA) method, involving the differentials of the measurable optical constants of the surface, it is possible to find a well-defined pair of incident angles to perform the measurement. Without a measurement error analysis, there would be no way of knowing what the absolute measurement uncertainty is or which angles of incidence could provide optimum measurement conditions. As in the case of single angle of incidence measurement where we were able to select an optimum angle of incidence to assure the highest measurement accuracy, the dual angle of incidence measurement also predicts optimum angles of incidence. It was found that in the case of single angle of incidence ellipsometry the principal angle of incidence can sharply define the optimum angle for measuring bare substrates and very thin films on a substrate. Likewise, for the dual angle of incidence measurement, there can also be two sharply defined angles for certain sample surface models. Here we present a dual angle ellipsometric measurement of the real part of the refractive index of a silicon substrate at the wavelength of 632.8 nm. A silicon dioxide film thickness between 125 and 150 nm and the two angles of incidence, 68 and 72 deg, optimized the measurement.

*600,844*
**PB86-202447** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Center for Electronics and Electrical Engineering Technical Publication Announcements, Covering Center Programs, April - June 1984 with 1984 CEEE Events Calendar,**
J. F. Mayo-Wells. Aug 84, 16p NBSIR-84/2927

Keywords: *Electronics, *Electrical engineering, Documents, Standards, Abstracts, Research projects, Semiconductors(Materials), Metrology, Signal processing.

The first issue of a quarterly abstract journal covering the work of the National Bureau of Standards Center for Electronics and Electrical Engineering. The issue of the Center for Electronics and Electrical Engineering Technical Publication Announcements covers the second quarter of calendar year 1984. Abstracts are provided by technical area for papers published the quarter.

*600,845*
**PB86-202553** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Effects of Phosphorus Contact Doping and Sheet Resistance Variations on Al/Si Interfacial Contact Resistance.**
Final rept.,
J. A. Mazer, L. W. Linholm, D. Pramanik, S. Tsai, and A. N. Saxena. 1983, 4p
Sponsored by Institute of Electrical and Electronics Engineers, Inc., Rochester, NY. Rochester Section.
Pub. in Proceedings of the Custom Integrated Circuits Conference, Rochester, NY., May 23-25, 1983, p291-294.

Keywords: *Integrated circuits, Semiconductor doping, Additives, Contacting, Reliability, Silicon, Aluminum, Phosphous, Metallizing, *Contact resistance, Very large scale integration.

The effects of phosphorus-contact doping and sheet resistance variations on interfacial contact resistance R sub C and on interfacial layer uniformity are investigated using a microelectronic test structure and electrical measurement method. Measurement results indicate that phosphorus-contact doping lowers the value of R sub C by as much as a factor of two without sacrificing the uniformity of the interfacial layer. The specific contact resistance is shown to be approximately directly proportional to the sheet resistance of the silicon in the contact window.

*600,846*
**PB86-210549** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Washington, DC.
**Center for Electronics and Electrical Engineering Technical Publication Announcements: Covering Center Programs, April-June 1985 with 1986 CEEE Events Calendar,**
E. J. Walters. Jan 86, 13p NBSIR-86/3310
See also PB86-201290.

Keywords: *Electronics, *Electrical engineering, Documents, Standards, Abstracts, Research projects, Semiconductors(Materials), Metrology, Signal processing.

This is the fifth issue of a quarterly publication providing information on the technical work of the National Bureau of Standards Center for Electronics and Electrical Engineering. The issue of the Center for Electronics and Electrical Engineering Technical Publication Announcements covers the second quarter of calendar year 1985. Abstracts are provided by technical area for papers published this quarter.

*600,847*
**PB86-213147** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Calibration of Aspirator-Type Ion Counters and Measurement of Unipolar Charge Densities.**
Final rept.,
M. Misakian, R. H. McKnight, and C. Fenimore. May 86, 77p NBS/TN-1223
Also available from Supt. of Docs as SN003-0003-02732-4.

Keywords: *Calibrating, Power transmission lines, Measurement, *Ion counters, *Ion density, *Ion detection, HVDC systems.

The characterization of a parallel plate apparatus which can produce a unipolar ion density that is suitable for calibrating aspirator-type ion counters operating in the ground plane is described. The influence of a dc electric field, air motion, Coulomb repulsion and diffusion on the transport of ions into the ion counter are examined to determine their effects on instrument calibration and measurements in the vicinity of high voltage dc transmission lines. An ion density which is known with an uncertainty of less than + or - 9% is used to check the performance of an ion counter with and without a duct at its entrance. The results of laboratory measurements of ion density under a monopolar high voltage line, which complement the studies with the parallel-plate apparatus, are also described.

*600,848*
**PB86-227410** PC **A07**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Design, Evaluation, and Use of a Reverberation Chamber For Performing Electromagnetic Susceptibility/Vulnerability Measurements.**
Technical note,
M. L. Crawford, and G. H. Koepke. Apr 86, 149p NBS/TN-1092
Also available from Supt. of Docs as SN003-003-02734-1. Sponsored by Naval Surface Weapons Center, Dahlgren, VA., and Rome Air Development Center, Griffiss AFB, NY.

Keywords: *Test facilities, Reverberation, Electomagnetic radiation, Vulnerability, Electromagnetic susceptibility, Reverberation chambers.

The report presents the results of work at the National Bureau of Standards, Boulder, Colorado, to carefully evaluate, document, develop (when necessary), and describe the methodology for performing radiated susceptibility/vulnerability measurements using a reverberation chamber. The report describes the reverberation chamber theory of operation, evaluation, functional operation, and use for performing immunity measurements. It includes an estimate of measurement uncertainties derived empirically from test results and from comparisons with anechoic chamber measurements. Finally, it discusses the limitations and advantages of the measurement technique to assist potential users in determining the applicability for the technique to their electromagnetic compatibility (EMC) measurement needs.

*600,849*
**PB86-229358** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Josephson Series Array Voltage Standard at One Volt.**
Final rept.,
C. A. Hamilton, R. L. Kautz, and F. L. Lloyd. 1985, 7p
Pub. in Proceedings of NCSL 1985 Workshop and Symposium, Boulder, CO., July 15-18, 1985, p71-77.

Keywords: *Josephson junctions, *Standards, Superconductivity, Substrates, Silicon, *Voltage standards.

Josephson voltage standards have long been limited by their low 1-10 mV output level. A new method for operating 1000 or more Josephson junctions in series has produced a practical standard at the one volt level. The junction array is in the form of a microstrip which is finline coupled to a waveguide at one end and is terminated at the other end. The whole circuit is fabricated on a 6 by 12 mm silicon substrate. With applied radiation at 72 GHz, the junction array produces up to 8000 quantized levels at the voltages nhf/2e. (In the United States 2e/h has an assigned value of 483593.420 GHz/V(NBS)). Any voltage from 0.1 to 1.2 volts can be obtained by selecting the level, n, and fine tuning the frequency, f. The high output voltage eliminates the need for a voltage divider and greatly reduces errors due to thermal voltages. When fully evaluated, the new standard is expected to have a precision of a few parts in a billion.

*600,850*
**PB86-229366** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Practical Josephson Voltage Standard at 1 V.**
Final rept.,
C. A. Hamilton, R. L. Kautz, R. L. Steiner, and F. L. Lloyd. 1985, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Electron Device Letters, EDL-6, n12 p623-625 Dec 85.

Keywords: *Standards, *Josephson junctions, Superconductivity, Reprints, *Voltage standards.

A series array of 1484 pairs of Josephson junctions, biased by microwaves at 72 GHz, is demonstrated to provide stable quantized voltages at the 1 V level. The niobium/lead-alloy junctions used in the array are not affected by thermal cycling.

*600,851*
**PB86-229374** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Sensitive, High Frequency, Electromagnetic Field Probe Using a Semiconductor Laser in a Small Loop Antenna.**
Final rept.,
R. J. Phelan, D. R. Larson, and P. A. Simpson. 1985, 7p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers, San Diego, CA., August 20-23, 1985, v566 p300-306.

Keywords: *Electromagnetic fields, Microwaves, Semiconductor lasers, Loop antennas, Avalanche diodes, Photodiodes, *Probes(Electromagnetic), Laser applications, Optical fibers.

Using a loop antenna in series with a semiconductor laser, an optically coupled electromagnetic field probe has demonstrated sensitivities better than 3 microV/(m.(Hz to the 1/2 power)). The probes outside dimensions are equal to 5.7 x 5.7 x 1.3 cc. It can be used to measure fields with frequencies as high as 2 GHz. The dynamic range is estimated to exceed 6 orders of magnitude for incident microwave powers.

*600,852*
**PB86-231164** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Intrinsic and Extrinsic Noise Sources in an RF Biased R-SQUID (Resistive-SQUID).**
Final rept.,
H. Seppa, J. H. Colwell, and R. J. Soulen. 1983, 5p
Pub. in Proceedings of International Conference on Noise in Physical Systems (7th), and International Conference on 1/f Noise (3rd), Montpellier, France, May 17-20, 1983, p399-403.

Keywords: *Temperature measuring instruments, Josephson junctions, Cryogenics, *Noise thermometers, SQUID devices.

The authors have modelled the influence of external circuit noise on the performance of a resistive-SQUID noise thermometer. The predictions of the model are in such good agreement with experimental results that one can reduce their influence to such an extent that noise thermometry free of systematic errors may be conducted to the 0.1% level from 1 mK to 500 mK.

*600,853*
**PB86-231461** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Measurements of Unintentional Electromagnetic Emissions.**
Final rept.,
M. T. Ma, and G. H. Koepke. 1986, 2p
Pub. in Proceedings of the IEEE (Institute of Electrical and Electronics Engineers) 74, n1 p110-111 Jan 86.

Keywords: *Electromagnetic radiation, *Electromagnetic interference, Measurement, TEM cells.

A summary of a new method for determining the radiation characteristics of leakage from electronic equipment or other unintentional radiators of interference is presented. The theoretical background and specific measurement procedures for the method using a transverse electromagnetic cell are outlined. The theory and measurements have been verified in referenced work by the results of a simulated theoretical example and an experiment using a spherical dipole radiator. Mathematical analysis of the uncertainties in the final, extracted results when the experimental data are degraded by the background noise and measurement imperfections is also available.

*600,854*
**PB86-231610** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Optical Fiber Sensors for the Measurement of Pulsed Electric Currents.**
Final rept.,
G. W. Day, J. D. O. McFadden, L. R. Veeser, G. I. Chandler, and R. W. Cernosek. 1985, 9p
Sponsored by Department of Energy, Washington, DC., Sandia National Labs., Albuquerque, NM., and Bonneville Power Administration, Portland, OR.
Pub. in Guided Optical Structures in the Military Environment (AGARD-CPP-383), Istanbul, Turkey, September 23-27, 1985, p8-1-8-9 1985.

Keywords: *Electric current, *Electrical measurement, Fiber optics, *Electric pulses.

Recent progress in the design of fiber sensors for pulsed electric currents is reviewed. Several of the most useful sensor configurations are described and compared. Models are used to predict the transfer function of these sensors, their sensitivity to non-ideal fiber properties, particularly linear birefringence, and methods for overcoming these problems. Other recent research is examined to suggest the prospect for sensors with improved sensitivity and stability.

*600,855*
**PB86-238680** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Optically Pumped Small Cesium Beam Standards: A Status Report.**
Final rept.,
A. Derbyshire, R. E. Drullinger, M. Feldman, D. J. Glaze, and D. Hilliard. 1986, 4p
Pub. in Proceedings of Annual Symposium on Frequency Control (39th), May 29-31, 1985, Philadelphia, PA., p18-21 1986.

Keywords: *Frequency standards, Cesium, Optical pumping, Laser pumping.

The authors report on their project to study and to demonstrate the potential performance achievable in cesium beam frequency standards in which laser driven optical pumping is used for the atomic state selection and state detection in place of the conventional magnetic state selection. The beam tubes used have been derived from commercial devices. In the first unit the only functional change was a simple replacement of state selection magnets with optics. In a second unit, the magnetic shields and c-field have been extended to include the regions of optical pumping.

*600,856*
**PB86-238698** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Beam Reversal Experiment on NBS-6 (National Bureau of Standards) Primary Cs Standard Including Rabi Pulling Evaluation.**
Final rept.,
A. DeMarchi, G. D. Rovera, R. Drullinger, and D. A. Howe. 1986, 5p
Pub. in Proceedings of Annual Symposium on Frequency Control (39th), May 29-31, 1985, Philadelphia, PA., p3-7 1986.

Keywords: *Frequency standards, Cesium.

An improvement in the evaluation of the Cs beam primary frequency standard NBS-6 is being attempted through a reevaluation of Rabi pulling using a recently published theory. Time of flight distribution measurements and frequency measurements at various C-field values have been performed in both beam directions. This allows the authors to model Rabi pulling and hence more clearly study other systematic effects.

*600,857*
**PB86-238706** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Recirculating Oven for Atomic Beam Frequency Standards.**
Final rept.,
R. E. Drullinger, D. J. Glaze, and D. B. Sullivan. 1986, 5p
Sponsored by Space Div., Los Angeles AFS, CA.
Pub. in Proceedings of Annual Symposium Frequency Control (39th), May 29-31, 1985, Philadelphia, PA., p13-17 1986.

Keywords: *Frequency standards, Atomic beams, Ovens.

The paper describes a simple recirculating oven which produces an atomic beam which can be better collimated than that from a conventional oven with equivalent collimation ratio. The oven is spill proof and requires only modest power for operation. Under suitable conditions the total beam flux can be significantly less than for conventional cesium ovens. This translates into more efficient use of the cesium charge and less contamination of the beam tube.

*600,858*
**PB86-239290** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Current NBS Metrology Capabilities and Limitations at Millimeter Wave Frequencies.**
Final rept.,
G. R. Reeve, and C. K. S. Miller. 1985, 13p
Pub. in Precision Measurements Association Newsnotes 2, p55-67 1985.

Keywords: *Metrology, Millimeter waves, Extremely high frequencies, Standards, Reprints, National Bureau of Standards.

The National Bureau of Standards (NBS) establishes national artifact standards and provides a metrology base for U.S. industry and technology. In the millimeter wave frequency spectrum, NBS has not established all of the required metrology to meet the needs of industry or government for this technology. It is the intent of the paper to describe the technical demands of responding to the challenges of millimeter wave technology.

*600,859*
**PB86-240777** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Fluorescent Light Shift in Optically Pumped Cesium Standards.**
Final rept.,
J. Shirley. 1986, 2p
Pub. in Proceedings of Annual Symposium on Frequency Control (39th), May 29-31, 1985, Philadelphia, PA., p22-23 1986.

Keywords: *Frequency standards, Cesium, Optical pumping.

The authors have calculated the light shift in an optically pumped cesium beam frequency standard caused by fluorescence co-propagating with the

atomic beam. Both scalar and tensor contributions are included to give the dependence on light polarization. The results provide design criteria for proposed new standards.

*600,860*
**PB86-247608** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Center for Electronics and Electrical Engineering Technical Publication Announcements Covering Center Programs, October to December 1985 with 1986 CEEE Events Calendar,**
E. J. Walters. Jul 86, 28p NBSIR-86/3424
See also PB86-201290.

Keywords: *Electronics, *Electrical engineering, Semiconductor devices, Metrology, Signal processing, Bibliographies.

This is the seventh issue of a quarterly publication providing information on the technical work of the National Bureau of Standards Center for Electronics and Electrical Engineering. This issue of the Center for Electronics and Electrical Engineering Technical Publication Announcements covers the fourth quarter of calendar year 1985. Abstracts are provided by technical area for papers published this quarter.

*600,861*
**PB87-102489** PC **A09**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Electromagnetic Compatibility and Interference Metrology,**
M. T. Ma, and M. Kanda. Jul 86, 180p NBS/TN-1099
Also available from Supt. of Docs as SN003-003-02760-0.

Keywords: *Electromagnetic compatibility, *Electromagnetic interference, *Metrology, Measurement.

The material included in the report is intended for a short course on electromagnetic compatibility/interference (EMC/EMI) metrology. The entire course is presented in nine chapters with the introductory part given as Chapter 1. The particular measurement topics to be covered are: (i) open sites (Chapters 2 and 6), (ii) transverse electromagnetic cells (Chapter 3), (iii) techniques for measuring the electromagnetic shielding of materials (Chapter 4), (iv) anechoic chambers (Chapter 5), and (v) reverberating chambers (Chapter 8). In addition, since small probe antennas play an important role in some of the EMC/EMI measurements covered herein, a separate chapter on various probe systems developed at NBS is given in Chapter 7. Selected contemporary EMI topics such as the characterization and measurement of a complex EM environment, interferences in the form of out-of-band receptions to an antenna, and some conducted EMI problems are also briefly discussed (Chapter 9).

*600,862*
**PB87-104923** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Quench Detector Circuit for Superconductor Testing.**
Final rept.,
W. P. Dube, and L. F. Goodrich. Apr 86, 3p
Sponsored by Department of Energy, Washington, DC.
Pub. in Review of Science Instruments 57, n4 p680-682 Apr 86.

Keywords: *Superconductors, Reprints, *Quench detectors, Critical current.

A quench detector is a device that interrupts the flow of current through a superconductor in the event the superconductor reverts to the normal, resistive state. The new design has adjustable filtering and sensitivity. The input is well isolated from the output, eliminating any possible ground loop through the detector. It also has excellent noise immunity. A detector has operated with no false trips for more than two years, detecting hundreds of quenches.

*600,863*
**PB87-104931** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Annealing of Bend-Induced Birefringence in Fiber Current Sensors.**
Final rept.,
G. W. Day, and S. M. Etzel. 1985, 4p
Sponsored by Department of Energy, Washington, DC.
Pub. in International Conference on Integrated Optics and Optical Fibre Communication (5th) - Technical Digest, v1 p871-874, Venice, Italy, 1-4 Oct 85.

Keywords: *Ammeters, *Fiber optics, *Birefringence, Electric current, Magnetic fields, Magnetic measurement, Detectors, Faraday effect, *Optical fibers.

The bend-induced linear birefringence in coils of single mode optical fiber has been greatly reduced by annealing. This should allow the construction of electric current sensors that are much more compact and potentially more sensitive than previously possible.

*600,864*
**PB87-106027** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Performing EM (Electromagnetic) Susceptibility/Vulnerability Measurements Using a Reverberation Chamber.**
Final rept.,
M. L. Crawford, and G. H. Koepke. 1986, 8p
Pub. in EMC EXPO 86 International Conference on Electromagnetic Compatibility, Washington, DC., June 16-19, 1986, pT28.7-T28.14.

Keywords: *Electromagnetic compatibility, Measurement, Vulnerability, *Electromagnetic susceptibility, Reverberation chambers.

The paper discusses the design, evaluation, and use of a reverberation chamber for performing electromagnetic susceptibility (EMS) measurements of electronic equipment. Included are brief descriptions of the test procedures, application advantages and limitations, some EMS test results, intrepretation of test results relative to free-space test methods, and an estimate of measurement uncertainties.

*600,865*
**PB87-106159** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**National Bureau of Standards Josephson Array Voltage Standard.**
Final rept.,
C. A. Hamilton, R. L. Kautz, and F. L. Lloyd. 1986, 2p
Pub. in Proceedings of 1986 Conference on Precision Electromagnetic Measurements, Gaithersburg, MD., June 23-27, 1986, p108-109.

Keywords: *Josephson junctions, *Standards, *Voltage standards, *Calibration standards, Josephson effect.

A Josephson voltage standard based on a series array of 2076 junctions is described. With a 15 mW input at 96 GHz, the array produces 15,000 quantized levels between -1.5 and 1.5 V. Initial results on high precision comparisons with a Zener reference standard are given.

*600,866*
**PB87-106373** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Pulse and Time-Domain Measurements.**
Final rept.,
R. A. Lawton, S. M. Riad, and J. R. Andrews. 1986, 5p
Pub. in Proceedings of the Institute of Electrical and Electronics Engineers 74, n1 p77-81 Jan 86.

Keywords: *Time domain, Measurement, Reviews, Pulses.

A review of the state of the art and science of pulse parameter measurements is given including recent advances in the use of real-time oscilloscopes, waveform recorders, equivalent time sampling oscilloscopes, and counter timers in the measurement of repetitive and single transient signals. Recent advances in the use of artifact waveform standards and modern signal analysis techniques to compensate for measurement distortion are highlighted. The formation and progress of an IEEE committee which is developing a performance standard for waveform recorders is also described.

*600,867*
**PB87-107355** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Test of the Quantum Hall Effect as a Resistance Standard.**
Final rept.,
M. E. Cage, R. F. Dziuba, and B. F. Field. 1985, 3p
Pub. in IEEE Transactions on Instrumentation and Measurement IM-34, n2 p301-303 Jun 85.

Keywords: *Standards, *Electrical resistance, Electrical measurement, Hall effect, Reprints.

The paper demonstrates that the quantum Hall effect can be used to monitor a laboratory unit of resistance. A 6,453.2 ohms room temperature reference resistor was calibrated relative to two quantum Hall effect devices with a 0.017 ppm (1 sigma) uncertainty for each one hour measurement period. The accuracy was acheived by correcting for a measurement system offset error and for the temperature dependences of each quantum Hall device. Hamon series-parallel resistor networks were then used to calibrate the 6,453.2 ohms resistor in terms of the five one ohm resistors which comprise the NBS ohm. The total 1 sigma accuracy for the transfer between the quantum Hall devices and the one ohm resistors was 0.047 ppm.

*600,868*
**PB87-108676** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Estimation of True Power Ratios in Six-Port Network Analyzers Using Diode Detectors.**
Final rept.,
D. R. Holt, and C. S. Hoer. Dec 85, 6p
Pub. in IEEE Transactions on Instrumentation and Measurement IM-34, n4 p558-563 Dec 85.

Keywords: *Network analyzers, Estimating, Detectors, Diodes, Reprints.

A model for detector nonlinearity is included in the determination of six-port parameters without using additional standards. A computer simulation was performed assuming that the true power into each six-port detector is related to the power observed by the detector. Simultaneous estimation of the six-port and detector parameters is accomplished through a nonlinear least squares algorithm. Results of the simulation compare Gamma computed from corrected power readings and Gamma calculated from observed power readings.

*600,869*
**PB87-110060** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Discussion of 'Four-Terminal Impedance Current Transformer Bridge with Resistive Ratio Arm' by Franco Castelli.**
Final rept.,
O. Petersons, and T. M. Souders. 1979, 2p
Pub. in Institute of Electrical and Electronics Engineers Transactions on Power Apparatus and Systems PAS-98, n3 p980-981 May/Jun 79.

Keywords: *Impedance bridges, *Electrical impedance, Current transformers, Electrical measurement, Reprints.

The advantages and disadvantages of a measurement technique for low value 4-terminal impedances is discussed. The method uses current transformer scaling and mixed ratio arms.

*600,870*
**PB87-110128** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Electromagnetic Shielding Effectiveness: Measurement Techniques and Interpretations.**
Final rept.,
P. F. Wilson, and M. T. Ma. 1986, 14p
Pub. in Institute of Electrical and Electronics Engineers Regional Conference and Exhibition on Electromagnetic Compatibility, Anaheim, CA., February 6, 1986, p1-14.

Keywords: *Electromagnetic shielding, Effectiveness, Measurement, Insertion loss.

A material's shielding capability is generally measured in terms of insertion loss: the field reduction between a transmitter and a receiver achieved by introducing the shield material. Ambiguities often arise when one attempts to interpret specific measurement results. Insertion loss data depend not only on the shield materi-

al tested, but also on the measurement procedure and other parameters such as the antenna types (both transmitting and receiving) used and their positioning, the incident waveform and its wave impedance, transient effects, and the contact resistance between the test material and its mount, if any.

*600,871*
**PB87-110136** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Methods for Measuring the Near-Field and Far-Field Shielding Effectiveness of Materials.**
Final rept.,
P. F. Wilson, and M. T. Ma. 1986, 6p
Pub. in EMC EXPO '86, Washington, DC., June 16-19, 1986, pT28.1-T28.6.

Keywords: *Electromagnetic shielding, Far field, Measurement, TEM cells, Near field.

Techniques for measuring the shielding effectiveness of materials are investigated. Specific approaches considered are coaxial transmission line holders and the use of a time-domain signal for simulating plane wave shielding performance, and the dual TEM cell and an apertured TEM cell in a reverberation chamber for the simulation of near-field shielding capability. The advantages and limitations of each technique are summarized.

*600,872*
**PB87-110144** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Simple Approximate Expressions for Higher Order Mode Cutoff and Resonant Frequencies in TEM (Tranverse Electromagnetic) Cells.**
Final rept.,
P. F. Wilson, and M. T. Ma. 1986, 6p
Pub. in Institute of Electrical and Electronics Engineers Transactions on Electromagnetic Compatibility EMC-28, n3 p125-130 Aug 86.

Keywords: Resonant frequency, *TEM cells.

Simple approximate expressions for determining the cutoff frequencies of the first few higher order modes and the associated resonant frequencies in transverse electromagnetic (TEM) cells are presented. Both symmetric (seven TE and two TM modes) and asymmetric (three TE modes) cells are discussed.

*600,873*
**PB87-115408** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Uncertainty Charts for RF and Microwave Measurements.**
Final rept.,
R. A. Kamper. 1986, 6p
Pub. in Proceedings of the Institute of Electrical and Electronics Engineers 74, n1 p27-32 Jan 86.

Keywords: *Electrical measurement, *Calibrating, Radio frequencies, Microwave frequencies, Reprints, US NBS, Uncertainty.

The scope of the calibration services for electrical quantities in the range of frequency from 0 to 100 GHz that are available from the National Bureau of Standards is discussed briefly in a historical context. Some plans for improved services that will be available in the near future are noted. Charts showing the variation of uncertainty with magnitude over the full range of the respective calibration services are presented.

*600,874*
**PB87-121356**
(Order as PB87-121315, PC **A04**/MF **A01**)
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Possible Changes in the U.S. Legal Units of Voltage and Resistance,**
B. N. Taylor. 31 Jul 86, 7p
Included in Jnl. of Research of the National Bureau of Standards, v91 n5 p299-305 Sep-Oct 86.

Keywords: *Standards, *Units of measurement, *Quantum Hall effect, *Josephson effect, *Volt, *Ohm, *Voltage standards, *Resistance standards, International system of units.

The Consultative Committee on Electricity of the International Committee on Weights and Measures is considerding adopting sometime in the future (1) a new value for the Josephson frequency-voltage ratio 2e/h (e is the elementary charge and h is the Planck constant) and (2) a value for the quantized Hall resistance RH=h/e(2). Both values are to be chosen as consistent with their International System of Units (SI) values as possible and would be used by every national standards laboratory which employs the Josephson and quantum Hall effects to define and maintain their national or legal units of voltage and resistance. Based on current knowledge, this would lead to an increase in the U.S. Legal Volt of about nine parts-per-millin (ppm) and an increase in the U.S. Legal Ohm of about 1.5 ppm. It is the purpose of the paper to review in some detail the basis for these proposed and potentially significant changes.

*600,875*
**PB87-125761** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Electromagnetic Radiation Test Facilities Evaluation of Reverberation Chambers Located at NSWC (Naval Surface Weapons Center), Dahlgren, Virginia,**
M. L. Crawford, and G. H. Koepke. Jun 86, 43p NBSIR-86/3051
Sponsored by Naval Surface Weapons Center, Dahlgren, VA. Dahlgren Labs.

Keywords: Electromagnetic shielding, Vulnerability, *Reverberation chambers, Electromagnetic susceptibility, Naval Surface Weapons Center.

The facilities were developed by the NSWC for use in measuring and analyzing the electromagnetic susceptibility/vulnerability (EMS/V) of weapon systems and the shielding effectiveness of enclosures and shielding materials. A brief description of each facility is given including the instrumentation used for performing the evaluation and calibration of the facilities by the National Bureau of Standards (NBS). Conclusions given indicate that the NSWC chambers can be used at frequencies down to approximately 150 MHz. Estimates are given of the measurement uncertainties derived empirically from the test results.

*600,876*
**PB87-134367** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Evaluation of Off-Axis Measurements Performed in an Anechoic Chamber.**
Technical note,
M. Kanda, and J. C. Wyss. Oct 86, 42p NBS/TN-1305
Also available from Supt. of Docs as SN003-003-02779-1.

Keywords: *Anechoic chambers, Waveguides, Ultrahigh frequencies, Horns.

Field strength versus distance from various source antennas is measured in a rectangular rf anechoic chamber on axes parallel to the boresight axis. An electrically small field probe is repeatedly scanned longitudinally away from the launch antenna and into the chamber. With each scan various parameters are changed, including: (1) horizontal and vertical position of the probe with respect to the center line of the launch antenna; (2) frequency; and (3) type of launch antenna. With the probe located 1 m off the center line and scanning between 2 and 6 m from the launch horn, the uncertainty due to being off the center line ranges from plus or minus 1 dB at 250 MHz to plus or minus 5.0 dB at 800 MHz and above. If the probe is within plus or minus 50 cm of center line, the uncertainty is no more than plus or minus 1.5 dB at 800 MHz; and, for plus or minus 25 cm from center line the uncertainty is further reduced to plus or minus 0.5 dB at 800 MHz.

*600,877*
**PB87-138384** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Design of the National Bureau of Standards Isotropic Magnetic Field Meter (MFM-10) 300 kHz to 100 MHz,**
J. E. Cruz, L. D. Driver, and M. Kanda. Oct 85, 57p NBS-TN-1085
Also available from Supt. of Docs as SN003-003-02770-7.

Keywords: *Magnetic fields, *Magnetic measurement, Electromagnetic interference, Field strength, Electromagnetic fields, Electric measuring instruments, Performance, Design, Microwave sensors, Near field.

A broadband magnetic field meter has been developed at the National Bureau of Standards (NBS) for the frequency range of 300 kHz to 100 MHz. The isotropic antenna unit consists of three mutually orthogonal loops, each 10 cm in diameter. The magnetic field probe described in the paper has a measurement range of 0.1 to 30 A/m. The readout of the meter is in terms of the Hermitian or 'total' magnitude of the magnetic field strength which is equal to the root-sum-square value of the three orthogonal magnetic field components at the measurement point. This magnetic field meter is nearly isotropic over its dynamic range. The electronic circuitry of the meter obtains the total magnitude of all field polarizations for all cw signals in the entire frequency band. The sensor is isotropic and is well suited for measuring the near field of an emitter, including regions of multiple reflections and standing waves. The meter can be used to monitor either the plane wave fields in the far zone of a transmitter, or the complicated fields very close to an rf leakage source. The report describes the design, performance and operating instructions for the MFM-10.

*600,878*
**PB87-140273** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Technical Publication Announcements Covering Center Programs, January to March 1986,**
E. J. Walters. Nov 86, 24p NBSIR-86/3486
See also PB86-247608.

Keywords: *Electronics, *Bibliographies, Semiconductor devices, Metrology, Integrated circuits, Signal processing, Antennas, Fiber optics, Lasers, Microwaves, Superconductors, Electromagnetic interference, Electric power, Abstracts.

This is the eighth issue of a quarterly publication providing information on the technical work of the National Bureau of Standards Center for Electronics and Electrical Engineering. The issue of the Center for Electronics and Electrical Engineering Technical Publication Announcements covers the first quarter of calendar year 1986. Abstracts are provided by technical area for papers published this quarter.

*600,879*
**PB87-140729** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Handbook for Operation and Maintenance of an NBS (National Bureau of Standards) Multisensor Automated EM (Electromagnetic) Field Measurement System,**
W. D. Bensema, G. H. Koepke, and H. W. Medley. Oct 86, 70p NBSIR-86/3056

Keywords: *Electromagnetic fields, *Handbooks, Detectors, Operation, Maintenance, Automation, Microcomputers, Computer programs, *Electromagnetic measurement, Computer applications, Hewlett-Packard computers.

A system is described that monitors and collects electromagnetic (EM) field strength information at five (optionally 10) locations simultaneously. The system has two modes of operation: (1) for sampling EM fields that are stationary for times of the order of 200 ms, and (2) for sampling changing EM fields with a system resolution of 10 microsec. Sensing elements for Mode 1 consist of three electrically short orthogonal dipoles mounted together, single dipole elements, or small loop antennas. Each element feeds a separate data input channel for a total of 15 (optionally 30) channels. Rf energy is converted to dc by a diode detector at each dipole. Mode 2 sensors will be diode detectors driven by broadband antennas. Real time system data processing includes calculation of field strength based on probe calibrations and processing of resultant data to satisfy measurement goals.

# ENERGY

## Batteries & Components

*600,880*
**PATENT-4 576 882** Not available NTIS
Department of the Navy, Washington, DC.
**Polyethylene Imine-Metal Salt Solid Electrolyte.**
Patent,
G. T. Davis, C. K. Chiang, J. M. Antonucci, and T. Takahashi. Filed 28 Feb 85, patented 19 Mar 86, 8p PB86-183530, PAT-APPL-6-706 811
Supersedes AD-D011 678.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Patents, *Solid electrolytes, *Electric batteries, Imines, Metals, Electrolytes, Polymers, Salts, Polyethylene.

The invention is a solid polymer electrolyte having (a) a matrix of linear poly(ethylene imine) having the formula (-CH2CH2NH-)n; and (b) a metal salt which is LiI, LiClO4, NaI, NaBr, KI, CsSCN, AgNO3, CuCl2, CoCl2, or Mg(ClO4)2, wherein the salt is dissolved in and distributed throughout the poly(ethylene imine) matrix and from more than zero to 0.10 moles of salt are used per mole of monomer repeat unit, -CH2CH2NH-.

## Electric Power Transmission

*600,881*
**PB86-231156** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Discussion of 'A Fast Response Impulse Voltage Measuring System for Testing of Gas Insulated Substations Equipment'.**
Final rept.,
R. H. McKnight. 1986, 1p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Power Delivery PWRD-1, n3 p47 Jul 86.

Keywords: *Electrical measurement, High voltage, Substations, Frequency response, Step response, Reprints.

The contribution is a discussion of a technical paper presented at the winter meeting of the Power Engineering Society, IEEE. It questions some of the authors assumptions, and references other applications of the measurement method described.

*600,882*
**PB87-131884** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Calibration of Test Systems for Measuring Power Losses of Transformers.**
Final rept.,
S. P. Mehta, and O. Petersons. 1986, 9p
See also PB86-132032.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Power Delivery PWRD-1, n4 p215-223 Oct 86.

Keywords: *Power transformers, *Power loss, Electrical measurement, Power factor, Calibrating, Reprints, Test methods.

Two years of development work by ASEA Electric, under the auspices of the Industrial Research Associate Program of the National Bureau of Standards has resulted in a verifiable method of determining overall accuracy of test systems used in the measurement of transformer losses. The technical achievement is important to the industry because of the present trend towards lower power factors which makes loss measurements exceedingly difficult with desirable test system accuracy that is traceable. The technical details of the work are presented in NBS Technical Note 1204 (over 100 page document). The intent of the IEEE paper is to present the basic principles embodied in the Technical Note. A calibration system for accuracy verification and alignment of test systems is described. Methodologies and data for evaluating accuracy of test systems are summarized.

## Energy Policies, Regulations & Studies

*600,883*
**PB86-163458** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**New Software Aids Life Cycle Costing of Energy Conservation Projects.**
Final rept.,
R. T. Ruegg, and S. R. Petersen. Sep 85, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in Heating/Piping/Air Conditioning 57, n9 p79-87 Sep 85.

Keywords: *Buildings, Reprints, *Computer software, *Life cycle costs, *Energy conservation, *Computer applications.

The article discusses briefly recent trends in computer software used in the building design process, and examines a new computer program for evaluating the life-cycle costs of alternative building designs and systems against this general perspective. The use of the Building Life-Cycle Cost (BLCC) computer program is illustrated in a case example, and its advances and limitations are noted. The point is made that though the move is towards expert systems, at this stage, expert knowledge on the part of the user continues to be required.

*600,884*
**PB86-199957** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Measurement of Temperature, Humidity, and Fluid Flow.**
Final rept.,
C. W. Hurley. Mar 86, 16p
Pub. in Proceedings of National Workshop - Field Data Acquisition for Building and Equipment Energy-Use Monitoring, Dallas, TX., October 16-18, 1985, p43-58 1986.

Keywords: *Temperature measuring instruments, *Measuring instruments, Humidity, Fluid flow, Temperature, Calibrating, Maintenance, Reprints.

Laboratory and field experience, and surveys, have clearly indicated that computerized laboratory and field tests and HVAC installations enhanced with Energy Management and Control Systems (EMCS) often experience problems related to the accuracy and reliability of the system instrumentation. The paper is being presented to call attention to only a few of the many neglected characteristics of instrumentation used in EMCS that have been found in the field to be the basic cause of problems in EMCS in new and existing installations. The characteristics of some of the available temperature, moisture, and flow monitoring instrumentation pertaining to EMCS application will be presented followed by typical problems encountered in interfacing various monitoring and control instrumentation with computer controlled systems.

## Fuel Conversion Processes

*600,885*
**DE85013673** PC **A08**/MF **A01**
National Bureau of Standards, Washington, DC. Metallurgy Div.
**Evaluation of the Performance of Materials and Components Used in the CO sub 2 Acceptor Process Gasification Pilot Plant.**
Final rept.,
R. C. Dobbyn, H. M. Ondik, W. A. Willard, W. S. Brower, and I. J. Feinberg. Apr 78, 169p DOE/ET/10253-T1
Contract AC01-76ET10253

Keywords: *Carbon Dioxide Acceptor Process, *Coal Gasification Plants, Alloys, Experimental Data, Flowsheets, Lignite, Materials, Performance, Pilot Plants, Recommendations, Refractories, South Dakota, ERDA/010404, ERDA/360100, ERDA/360200.

This report addresses the performance of materials and components used in the operation of the Conoco Lignite Gasification Pilot Plant, located in Rapid City, South Dakota. Facts relating this performance over the five and one-half years of plant operation were acquired primarily from the plant operating records. Run reports, lists of shutdown work performed between runs, inspection reports and monthly reports to project sponsors were read and operating events were identified, classified and abstracted. In addition, other documents, generated over the life of the plant, were analyzed; these include the plant construction report, Conoco failure reports, annual reports and other memoranda. Several visits to the plant were made and discussions of some of the unique features of this plant were held on several occasions with Conoco and Stearns-Roger personnel. Performance histories and assessments of this performance have been given for all materials and components for which there was sufficient information contained in these plant records. Performance is summarized under each major component or class of components in the body of the report. A plan for sampling selected materials of construction, both metals and refractories, for laboratory analysis was submitted to plant management and project sponsors and resulted in a laboratory analysis limited to the refractory lining of the gasifier vessel. A report of the findings of this laboratory evaluation has been made an appendix to this report. Conclusions and recommendations for future efforts in developing performance information are given. 6 refs., 29 figs., 5 tabs. (ERA citation 10:035895)

*600,886*
**PB86-195609** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Free Radicals in Coal Conversion.**
Final rept.,
S. E. Stein. 1985, 32p
Pub. in Chem. Coal Convers., p13-44 1985.

Keywords: *Coal, *Free radicals, Pyrolysis, Kinetics, Reprints.

It is generally accepted that free radicals are the key reactive intermediates in thermal coal chemistry. This view is supported by the general observation that free-radical reactions control the pyrolysis chemistry of most organic substances. General kinetic features of coal liquefaction have also been used to support this view. A detailed consideration of the chemical structure of coal and its reaction products also strongly suggests that free-radical reactions control coal chemistry. The aromatic and hydroaromatic units found in coal tars and liquids and presumed to be dominant structures in coal itself are known to be very reactive toward free radicals. Moreover, resonance stabilized radicals derived from these structures are formed and react readily at coal decomposition temperatures. Methyl and hydroxyl substituents serve to increase the overall free-radical reactivity of the molecules to which they are attached.

*600,887*
**PB87-104220** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Viscosities and Densities of Selected Organic Compounds and Mixtures of Interest in Coal Liquefaction Studies.**
Final rept.,
Y. Oshmyansky, H. J. M. Hanley, J. F. Ely, and A. J. Kidnay. 1986, 10p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in International Jnl. of Thermophysics 7, n3 p500-608 1986.

Keywords: *Viscosity, *Density(Mass/volume), Thermophysical properties, Organic compounds, Xylene, Thiophene, Quinoline, Cresols, Reprints, *Coal liquefaction, Naphthalene/methyl, Tetralin, Tetrahydrofuran, Coal liquids.

Experimental measurements are presented for the density and viscosity of selected organic compounds and mixtures at ambient pressure (0.083 M Pa) and at temperatures of 298, 318, 338, and 358 K. The compounds studied were decalin, 1-methylnaphthalene, tetralin, m-xylene, tetrahydrofuran, thiophene, quinoline 2,6-lutidine, and m-cresol. Measurements were also made on three mixtures of the compounds decalin, 1-methylnaphthalene, tetralin, m-xylene, and m-cresol. The experimental results are compared with predictions made using a modified corresponding states procedure called TRAPP. The density predictions for the individual compounds and mixtures are good in all cases. For the viscosity, however, the predictions are in reasonable agreement with experiment only for nonassociating compounds and mixtures at reduced densities less than 3. These results suggest that TRAPP may prove very useful as a screening test to distinguish between nonassociating and highly associating mixtures. Such a test would be extremely useful when dealing with mixtures of unknown composition, such as coal liquids.

## Fuels

*600,888*
**PB83-195081** PC **A04/MF A01**
National Bureau of Standards, Washington, DC.
**Thermophysical Properties of Fluids for the Gas Industry.**
Annual rept. Jan-Dec 82,
Howard J. M. Hanley. 10 Jan 83, 70p GRI-82/0042
Contract GRI-5014-361-0131

Keywords: *Thermophysical properties, *Gas industry, Gases, Liquids, Fuels, Technology, Natural gas, Liquefied natural gas, Coal, Heavy oils, Bituminous sands, Thermodynamic properties, Chemical feedstocks, Synthetic fuels.

To provide the gas and related industries with a data base and a means to predict the thermophysical properties of gases and liquids.

*600,889*
**PB84-216977** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Estimating Large Pool Fire Burning Rates.**
Final rept.,
V. Babrauskas. Nov 83, 11p
Pub. in Fire Technology, v19 n4 p251-261 Nov 83.

Keywords: *Flammable liquids, *Burning rate, Jet engine fuels, Predictions, Flame propagation, *Pool fires.

Data for predicting the burning rate and heat output of large pool fires (Diameter greater or equal to 0.2 m) are compiled and evaluated. Attention is also focused on areas where further research is most needed in order to improve predictability.

*600,890*
**PB86-162112** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**LNG (Liquefied Natural Gas) Property Data and Metrology Technology.**
Final rept.,
D. Mann, and J. A. Brennan. 1985, 10p
Sponsored by Groupe Internationale des Importateurs de Gas Natural Liquefie, and Southern California Gas Co., Los Angeles.
Pub. in Proceedings of the World Gas Conference (16th), Munich, West Germany, June 24-27, 1985, p1-10.

Keywords: *Liquefied natural gas, Chemical properties, Reviews, Physical properties, Technology, Measurement instrumentation, Tables(Data).

Results of National Bureau of Standards (NBS) research programs concerning Liquefied Natural Gas (LNG) are presented and reviewed. In addition to previously reported information on LNG materials and fluids property data in graphic format, these more recent programs provide information on combustion enthapies of the LNG components and mixtures for molecular weights of methane through the hexanes, real gas mixture densities, both measured and calculated and other thermophysical properties correlations, tabulations, and equations of state. The metrology of custody transfer is presented in context of previously completed NBS research programs dealing with LNG. These include LNG sampling and analysis, LNG density measurement both direct and calculated, liquid level instrumentation, ship and shore tank strapping and liquid flowmetering. Each of these measurement processes are examined for accuracy and precision. Propagation of error is presented with sample calculations and assessed for the various custody transfer situations such as ship tank unloading, pipeline flowmetering, shore tank storage and vaporization and gas flow measurements.

*600,891*
**PB86-193158** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Laboratory-Scale Controlled-Atmosphere Chamber for Use with Premium Coal Samples.**
Final rept.,
B. J. Filla, and J. E. Callanan. 1985, 4p
Pub. in Review of Scientific Instruments 56, p592-595 Apr 85.

Keywords: *Laboratory equipment, *Atmosphere control, Coal, Recirculating system, Reprints, *Controlled atmosphere chamber, Glove box.

The recent availability of premium coal samples makes it desirable to have the capability for working with these materials, in one's own laboratory, in an atmosphere which can be controlled. A controlled-atmosphere chamber, large enough to allow for processing samples yet small enough to fit easily in an ordinary laboratory, has been designed and fabricated. The overall cost of the controlled-atmosphere chamber was competitive with commercially available systems. The major advantages of the specific system include: convenient size and reversible design for use in a limited work space; incorporation of a full vacuum antechamber that minimizes loss of the working chamber purified atmosphere; and a recirculating system with a bypass valve arrangement allowing separate or combined operation of oxygen and moisture removal systems. The design features were combined to create a unique apparatus capable of both the specific use for which it was intended and general controlled-atmosphere chamber applications. Compatible modular-design work chambers could have been purchased from commercial vendors; however, it still would have been necessary to custom fabricate both the antechamber and recirculation system to meet the requirements of the anticipated experimental work.

*600,892*
**PB86-208386** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Gel Model for Coal.**
Final rept.,
R. A. MacDonald, and R. D. Mountain. 1985, 7p
Pub. in International Jnl. of Thermophysics 6, n6 p673-679 Nov 85.

Keywords: *Coal, Aggregates, Density functions, Density(Mass/volume), Thermodynamic properties, Gels, Reprints.

Coal is a sedimentary, organic 'rock' which is almost never in a state of thermal equilibrium. Because of its importance, the thermal properties of this ill-characterized substance are of great interest. Recent work has shown that coal has many of the characteristics of a gel-type structure. We have made this observation the basis for a model study of the thermal properties of a gel system, using the equation-of-motion method to determine the density of states for the system and, thereby, its heat capacity. The model has one of the essential features of a model of coal, namely, a porous structure. With a hexagonal close-packed lattice as the basis for our gel, we have calculated the frequency spectrum for several particle densities.

*600,893*
**PB86-208493** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Physical Properties of Pure Components of Natural Gas.**
Final rept.,
K. N. Marsh. 1986, 15p
Pub. in Gas Quality, p59-73 1986.

Keywords: *Natural gas, Physical properties, Combustion, Reprints.

The principal physical properties of components of natural gas that are of importance to the gas industry are those related to heating value and to volume. New recommendations for the heating values and molar volumes of components of natural gas and for their molar volumes are reported. These are based on a reassessment of the available experimental data.

*600,894*
**PB86-209673** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Comparison of Single Component Standards to Multi-Component Standards for Use in Analysis of Natural Gas.**
Final rept.,
G. C. Rhoderick, and E. E. Hughes. 1986, 9p
Pub. in Gas Quality, Proceedings of International Congress on Gas Quality-Specification and Measurement of Physical and Chemical Properties of Natural Gas, Groningen (Netherlands), April 22-25, 1986, p711-719.

Keywords: *Natural gas, *Standards, Simulation, Comparison, Gravimetric analysis.

The precise analysis of natural gas requires the identification and quantification of a large number of components. A simulated natural gas mixture consisting of methane and seven higher hydrocarbons together with nitrogen and carbon dioxide has been prepared. Thirty gaseous standards have been prepared by a gravimetric technique. These standards consist of several concentrations each of the single components and two standards containing all of the components. Analyses were performed on the simulated natural gas and on samples of natural gas. The analysis resulting from calibration with the binary standards was compared to analytical results obtained using the multi-component standards.

*600,895*
**PB86-232709** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**LNG (Liquefied Natural Gas) Densities for Custody Transfer.**
Final rept.,
R. D. McCarty. 1983, 3p
See also PB82-112574.
Pub. in Proceedings of International School of Hydrocarbon Measurement (58th), Norman, OK., April 12-14, 1983, p121-123.

Keywords: *Liquefied natural gas, *Density(Mass/volume), Densimeters, Standard reference materials, Numerical solution.

Work has been carried out over the past ten years at the National Bureau of Standards to provide alternate methods for the accurate determination of the density of liquefied n natural gas (LNG) that would serve as a basis for equitable custody transfer. A magnetic suspension densimeter was used to obtain density data for LNG components and their mixtures with a total uncertainty in density of less than 0.1%. These data were used to optimize and test mathematical models for LNG density calculations. Four mathematical models for the calculation of LNG densities have been optimized, tested, and compared.

*600,896*
**PB86-233269** PC **A15/MF A01**
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**LNG (Liquefied Natural Gas) Measurement: A User's Manual for Custody Transfer.**
Final rept.,
D. Mann. Jun 86, 327p NBSIR-85/3028
Color illustrations reproduced in black and white. Sponsored by Groupe Internationale des Importateurs de Gaz Natural Liquefie.

Keywords: *Liquefied natural gas, Density(Mass/volume), Measurement, Instruments, Data.

The LNG Measurement Manual will provide measurement engineers and others with a source of critically

evaluated basic physical property data, a description of recent relevant measurement research and detailed examples of several methods of establishing the quantity and quality of liquefied natural gas (LNG) as a commercial commodity at the custody transfer point of sale. The contents of the manual are edited condensations of published research on properties and measurement processes.

*600,897*
**PB87-104246** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Equation of State Model for Pure CO2 and CO2 Rich Mixtures.**
Final rept.,
J. F. Ely. 1986, 8p
Pub. in Proceedings of Annual Convention of the Gas Processors Association (65th), San Antonio, TX., March 1986, p185-192.

Keywords: *Carbon dioxide, *Equations of state, Mathematical models, Thermophysical properties, Reprints, *Enhanced oil recovery.

Enhanced oil recovery using carbon dioxide and associated carbon dioxide pipeline and gas processing interests have generated a great demand for accurate thermophysical property data for systems containing CO2. In an attempt to meet these demands, an experimental measurement and model development program has been undertaken at the National Bureau of Standards dealing with pure carbon dioxide and CO2 rich mixtures. The entire fluid range of conditions has been studied in the work but special attention has been paid to single phase properties such as densities and enthalpies in the near but supercritical region. In the report, a new equation of state for pure carbon dioxide and an accurate equation of state model for CO2 rich mixtures will be discussed.

*600,898*
**PB87-118097** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Tests of Models for Shear Viscosity Coefficients.**
Final rept.,
D. E. Diller, and L. J. van Poolen. 1985, 6p
Sponsored by Gas Research Inst., Chicago, IL., and Department of Energy, Washington, DC.
Pub. in High Temperatures-High Pressures 17, p139-143 1985.

Keywords: *Viscosity, *Gases, Density(Mass/Volume), Temperature, Reprints, Compressed gases.

Recent measurements of the dynamic shear viscosity of compressed and liquefied hydrocarbon gases are compared with a global extended corresponding states model. At densities approx less than 2.5 rho sub c, the measurements and model generally differ by less than 7%. At higher densities, however, the differences are substantially larger, and increase with increasing density. Our data for liquid isobutane are satisfactorily correlated by using the Hildebrand equation. A good correlation was found between the fluidities (viscosity) of the liquids examined and their mean molecular radius of gyration.

*600,899*
**PB87-128302** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**NBS (National Bureau of Standards)-Boulder Basic Gas Metering Project.**
Final rept.,
J. A. Brennan, B. R. Bateman, S. E. McManus, C. F. Sindt, and I. Vazquez. 1986, 8p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in American Gas Association 1986 Operating Section Proceedings, p773-780.

Keywords: *Gas flow, *Orifice meters, *Flowmeters, Laboratories, Flow measurement, Experimental data, Mass flow, Pipes, Comparisons, *Data bases, European economic community.

Recent developments in the multi-year gas flow measurement program include new experimental orifice meter coefficient data, an archival orifice meter data base, an interlaboratory comparison with flow facilities in the European Economic Community (EEC), and tests on five flow conditioners. The current status of these tasks is described and some examples are presented that may be useful in future revisions of the orifice flow measurement standard.

*600,900*
**PB87-132056** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Characterization of Refuse-Derived Fuel at Various Stages of Processing.**
Final rept.,
D. R. Kirklin, P. H. Decker, and E. S. Domalski. 1985, 7p
Pub. in Resour. Conserv. 11, n3-4 p255-261 1985.

Keywords: Sulfur, Chlorine, Separation, Calorimetry, Calorific value, Reprints, *Refused derived fuels, Municipal solid wastes.

The combustible fraction was separated from a municipal solid waste (MSW) sample from New Castle County, Delaware at the Bureau of Mines (BuM) pilot resource recovery plant in College Park, Maryland. The combustible fraction was collected at seven points after various stages of processing through air classifiers and trommels. The calorific value, moisture, ash, sulfur and chlorine contents were measured by NBS and BuM laboratories and the results analyzed to determine if these properties were characteristic of or altered by the type of processing that the refuse-derived fuel (RDF) had under gone. The NBS analysis concluded that some of the RDF properties are characteristic of or altered by the type of processing that the RDF had undergone. Air classifiers were very effective in separating the light components of RDF (i.e., paper and plastic films) from the heavier components of RDF. A trommel in the RDF separation scheme removes some of the undesirable characteristics of RDF, namely, the non-combustible, sulfur and chlorine containing components of RDF.

*600,901*
**PB87-141487** PC **A06**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Natural Gas Handbook,**
P. R. Ludtke. Aug 86, 109p NBSIR-86/3057
Sponsored by Air Force Engineering and Services Center, Tyndall AFB, FL.

Keywords: *Natural gas, Moisture content, Hydrogen sulfide, Concentration(Composition), Compressibility, Handbooks, Measuring instruments.

A Natural Gas Handbook has been prepared to help Air Force BCE personnel better understand the principles of metering and selling natural gas on an energy content basis. The various aspects of natural gas such as heating value, moisture content, and hydrogen sulfide content are discussed. The characteristics of the various types of meters currently used for flow measurements are given. The correct procedures for calculating gas utility bills, including compressibility corrections, are presented. The responsibility of the gas utility to periodically check the gas meter and instrument accuracy is discussed. A list of information that should appear on the gas utility bill is given, and the various methods of selling natural gas are discussed.

## Heating & Cooling Systems

*600,902*
**PB86-166279** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Rating Procedure for Mixed Air Source Unitary Air Conditioners and Heat Pumps Operating in the Cooling Mode,**
P. A. Domanski. Feb 86, 21p NBSIR-86/3301
Sponsored by Department of Energy, Washington, DC.

Keywords: *Air conditioners, *Heat pumps, *Ratings, Cooling.

A procedure is presented for rating split, residential air conditioners and heat pumps operating in the cooling mode which are made up of an evaporator unit combined with a condensing unit which has been rated under current procedures in conjunction with a different evaporator unit. The procedure allows calculation of capacity at the 95 degrees F rating point and seasonal energy efficiency ratio, SEER, without performing laboratory tests of the complete system.

*600,903*
**PB86-168267** PC **A17**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Modeling of a Heat Pump Charged with a Non-Azeotropic Refrigerant Mixture.**
Final rept.,
P. Domanski. Jan 86, 396p NBS/TN-1218
Also available from Supt. of Docs as SN003-003-02716-2. Sponsored by Electric Power Research Inst., Palo Alto, CA.

Keywords: *Heat pumps, *Refrigerants, Air conditioning, Vapor compression refrigeration cycle.

An analysis of the vapor compression cycle and the main components of an air-to-air heat pump charged with a binary non-azeotropic mixture has been performed for steady-state operation. The general heat pump simulation model HPBI has been formulated which is based on independent, analytical models of system components and the logic linking them together. The logic of the program requires an iterative solution of refrigerant pressure and enthalpy balances, and refrigerant mixture and individual mixture component mass inventories. The modeling effort emphasis was on the local thermodynamic phenomena which were described by fundamental heat transfer equations and equation of state relationships among material properties. In the compressor model several refrigerant locations were identified and the processes taking place between these locations accounted for all significant heat and pressure losses.

*600,904*
**PB86-192184** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Effect of a Time-Delayed Stack Damper on Off-Cycle Heat Losses for Residential Heating Equipment.**
Final rept.,
C. Park, D. A. Didion, and G. E. Kelly. 1983, 10p
Sponsored by American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA.
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 89, pt2A-2B p373-382 1983.

Keywords: *Heating equipment, Time lag, Delay circuits, Residential buildingss, Reprints, *Stack Damper.

Computer procedures were developed for modeling stack dampers with delayed operation between burner shut-off and damper closure. Correction factors for the time delay have been obtained and a quantitative theoretical rationale is used to evaluate the effect of the time delay on the seasonal efficiency of fossil fuel-fired residential heating equipment. Finally, an implementation procedure is outlined for incorporating this rationale into the existing DoE's furnace/boiler seasonal efficiency test and evaluation procedure.

*600,905*
**PB86-192416** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Wall and Ceiling Protection for Heating Appliances.**
Final rept.,
J. J. Loftus, and R. D. Peacock. 1985, 17p
Pub. in Fire Technology 21, n3 p213-229 Aug 85.

Keywords: *Fire protection, *Radiant heating, Stoves, Chimneys, Ceiling(Architecture), Walls, Building codes, Reprints, *Radiant heat transfer.

An evaluation was made of the effects of radiant heat transfer from hot stove and chimney pipes to unprotected and protected room walls and ceilings. Pipe surface temperatures were 350 degrees C (662 degrees F) for normal operation, and 400-450 C degrees C (752-842 degrees F) to simulate overfire conditions. Recommendations for model building code specifications for wall and ceiling protection are provided.

*600,906*
**PB86-203577** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Effect of Wall Mass on the Winter Heating Loads and Indoor Comfort: An Experimental Study.**
Final rept.,
D. M. Burch, D. F. Krintz, and R. S. Spain. 1984, 28p
Sponsored by American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA.

Pub. in Proceedings of 1984 Winter Meeting of the American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA., January 29-February 1, 1984, ASHRAE Transactions 90, Pt. 1B, p94-121.

Keywords: *Residential buildings, *Walls, Model tests, Comfort, *Energy conservation, Energy consumption, Heating load.

Six test buildings were extensively instrumented for measuring heating loads and indoor comfort. These test buildings were exposed to a winter heating season and an intermediate heating season. During the winter season, when some space heating was supplied each hour of test, measured heating loads were predicted with a steady-state heat-transfer model which did not include the effect of thermal mass. The indoor comfort was not affected by wall mass. During the intermediate heating season, when the indoor temperatures floated above the thermostat set temperatures during warm day periods, a significant thermal mass effect was observed. Heavyweight buildings were observed to consume less heating energy than comparable lightweight buildings having equivalent wall thermal resistance. The effect was greater when wall mass was positioned inside as opposed to outside wall insulation. Wall mass was observed to reduce considerably overheating during warm day periods, and thereby produce more comfortable indoor conditions.

*600,907*
**PB86-237104** PC **A07**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Verification of Public Domain Control Algorithms for Building Energy Management and Control Systems,**
W. B. May, and G. E. Kelly. Dec 85, 142p NBSIR-85/3285
Sponsored by Department of Energy, Washington, DC., and Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Control equipment, *Buildings, *Computer programs, Algorithms, Field tests, Heating, Ventilation, Air conditioning, *Energy management.

Software is an important component of building energy management and control systems (EMCS). The National Bureau of Standards developed and documented eight public domain EMCS supervisory control algorithms. The testing and verification of these eight algorithms are described in the report. The algorithms tested cover dry bulb and enthalpy economizer cycles, optimum and scheduled start/stop, duty cycling, demand limiting, outside air supply air reset, and demand supply air reset.

*600,908*
**PB86-247871** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Evaporation of a Water Droplet Deposited on a Hot High Thermal Conductivity Solid Surface,**
M. di Marzo, and D. D. Evans. Aug 86, 34p NBSIR-86/3384
Prepared in cooperation with Maryland Univ., College Park. Dept. of Mechanical Engineering.

Keywords: *Evaporative cooling, *Evaporation, Surfaces, Thermal conductivity, Sprinkler systems, Sprayers, *Water droplet.

A model is presented that predicts major features of the evaporation of water droplets deposited on a hot non-porous solid surface. In the temperature range of interest, nucleate boiling heat transfer is fully suppressed, hence the model is only concerned with the evaporative process. In the model, the solid material is assumed to have high thermal conductivity and diffusivity, so that the surface temperature under the water droplet can be considered uniform. The temperature of the portion of a larger solid surface covered by the liquid is calculated from the classic solution for contact temperature between two semi-infinite bodies.

*600,909*
**PB87-108619** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Proposed TC 4.7 Simplified Energy Analysis Procedures.**
Final rept.,
T. Kusuda, and I. Sud. 1982, 1p
Sponsored by Department of Energy, Washington, DC.
Pub. in American Society of Heat, Refrigeration, and Air Conditioning Engineers Transactions, v88 Pt2 p6 1982.

Keywords: Reprints, *Space HVAC systems, *Energy analysis, Energy conservation, Computer applications.

The general principle of a simplified energy analysis procedure suitable for use in a small engineering office with a desk-top or pocket calculator is developed for building energy conservation standards application. The procedure is based upon ASHRAE cooling load factor techniques for the load calculation, and standard psychrometric heat balance calculations for the HVAC system analysis and seasonal efficiency of equipment performance (which is found in the REAP methodology). The use of the procedure is illustrated for an office building with a VAV air distribution system connected to a centrifugal chiller and hot water boiler.

## Miscellaneous Energy Conversion & Storage

*600,910*
**PB86-213568** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Report of Tests on Joseph Newman's Device,**
R. E. Hebner, G. N. Stenbakken, and D. L. Hillhouse. Jun 86, 40p NBSIR-86/3405
Sponsored by Patent and Trademark Office, Washington, DC.

Keywords: *Power supplies, Electrical measurement, Electric converters, Efficiency, Power loss, Power, Signal generators, Spectrum analysis.

The report describes tests performed between March 1986 and June 1986 on a device submitted by Joseph Newman for testing at the National Bureau of Standards. The purpose of the testing was to determine if the output power of the device was greater than the input power.

*600,911*
**PB87-122610** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Methodology for the Evaluation of the Thermal Performance of Phase-Change Storage Materials.**
Final rept.,
J. W. Grimes, P. W. Brown, and L. Kaetzel. 1985, 5p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Testing and Evaluation 13, n6 p429-433 Nov 85.

Keywords: *Sodium sulfates, Heat measurement, Performance, Thermal cycling tests, Hydrates, Reprints, *Thermal storage, *Phase change materials.

A methodology to evaluate the response of phase change thermal storage materials to repeated thermal cycling is described. The methodology is based on the utilization of a thermal cycling device to simulate in-service conditions and an isoperibolic calorimeter to measure the thermal storage capacities of the phase change specimens. The thermal cycling device was designed to operate over a range of predetermined conditions including heating and cooling rates and maximum and minimum cycle temperatures. The design and operating characteristics of the device is described. Data obtained by investigating the Na2SO4 10H2O phase change system indicate that the methodology can be used to assess the performance and durability of phase change storage systems.

*600,912*
**PB87-128278** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Heats of Dehydration and Specific Heats of Compounds Found in Concrete and Their Potential for Thermal Energy Storage.**
Final rept.,
L. J. Struble, and P. W. Brown. 1986, 12p
Pub. in Solar Energy Materials 14, p1-12 1986.

Keywords: *Heat storage, *Concretes, Inorganic salts, Hydrates, Dehydration, Solar heating, Reprints, *Latent heat storage, Ettringite, Friedel's salt, Building materials.

Two classes of hydrated inorganic salts have been studied to assess their potential as materials for passive solar energy storage. The two classes of salt are typified by ettringite, a trisubstituted salt, and Friedel's salt, a monosubstituted salt, both of which are typically found in Portland cement concrete. The trisubstituted salts were studied to assess their potential for latent heat storage, utilizing a low-temperature dehydration reaction, and both classes were studied to assess their potential for sensible heat storage. Preliminary experiments indicate the dehydration of the trisubstituted salts is reversible, though additional tests are required. The thermal data demonstrate that the trisubstituted salts have potential as latent heat storage materials and both classes of salts have potential as sensible heat storage materials; furthermore, it is noted that the materials may be contained in conventional Portland cement concrete, making them particularly attractive for thermal energy storage.

## Solar Energy

*600,913*
**PB86-199965** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Results from the NBS (National Bureau of Standards) Passive Test Building: A Status Report.**
Final rept.,
B. M. Mahajan, and S. T. Liu. 1983, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Passive and Hybrid Solar Energy Program Update Conference, Washington, DC., September 26, 1983, p70-78.

Keywords: *Buildings, Data, Tests, *Passive solar cooling systems, *Passive solar heating systems, Solar architecture.

The National Bureau of Standards Passive Solar Test Building, constructed under the sponsorship of the U.S. Department of Energy, has been operational since October 1981. The test building has been constructed for the purpose of acquiring class A performance monitoring data for various passive systems under different experimental conditions. The report briefly describes the test building, instrumentation and data acquisition system, continuous air infiltration monitoring system and experimental work conducted in fiscal year 1983. The report contains representative data, and briefly describes the research activities planned for the future.

*600,914*
**PB86-201282** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Inorganic Compounds for Passive Solar Energy Storage - Solid-State Dehydration Materials and High Specific Heat Materials.**
Progress rept.,
L. Struble, and P. Brown. Apr 86, 71p NBSIR-86/3325
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: *Energy storage, Solar energy, Inorganic salts, Dehydration, Specific heat, Passive systems, Sensible heat storage.

Two classes of hydrated inorganic salts have been studied to assess their potential as materials for passive solar energy storage. The materials are part of the quaternary system CaO-A12O3-SO3-h2O and related chemical systems, and the two classes are typified by ettringite, a trisubstituted salt, and Friedel's salt, a monosubstituted salt. The trisubstituted salts were studied for their possible application in latent heat storage, utilizing a low-temperature dehydration reaction, and both classes were studies for their application in sensible heat storage. In order to assess their potential for energy storage, the salts have been synthesized, characterized by several analytical techniques, and thermal properties measured. The dehydration data of the trisubstituted salts vary somewhat with chemical composition, with the temperature of the onset of dehydration ranging from 6 degrees C to 33 degrees C, and enthalpy changes on dehydration ranging from 60 to 200 cal/g. Heat capacity is less variable with composition; values for the trisubstituted phases are 30 cal/g/degrees C and for the monosubstituted phases between 0.23 and 0.28 cal/g/degrees C.

*600,915*
**PB86-210226** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Convection between Zones with Non-Linear Temperature Distributions.**
Final rept.,
D. D. Hill, and B. M. Mahajan. 1986, 7p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Air Movement and Distribution Conference, Lafayette, IN., May 27-29, 1986, p109-115 May 86.

Keywords: *Convection, Heat transmission, Buildings, Doors, *Solar equipment.

Interzonal natural convection is an important process in the redistribution of thermal energy in passive solar enclosures. In the paper, interzonal natural convection in a two zone full scale building with non-linear zone temperature distributions is analyzed. Measurements of interzonal convection were taken in a doorway joining two rooms of the National Bureau of Standards Passive Solar Test Facility. A bernoulli interzonal air flow model based on isothermal zone temperatures is modified to account for the non-linear zone temperature distributions.

*600,916*
**PB86-244167** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Experimental and Analytical Investigation of Solar Radiant Flux Distribution on Interior Surfaces of a Sunspace,**
S. T. Liu. Mar 86, 26p NBSIR-86/3378
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: Solar radiation, Measurement, Experimental data, *Solar flux, Passive solar heating systems, SUNFLUX computer program.

The short wave solar radiant flux distribution inside a sun-space model with a large south opening was studied experimentally under clear sky conditions. Miniature photovoltaic pyranometer sensors responsive to short wave radiation were mounted at various locations on the interior surfaces of the enclosure. An NBS developed solar flux distribution program was tested against the experimental results and was found to give good agreement. The computer program can be used as a design tool for the evaluation of thermal storage location and solar physical properties of floor and walls in a passive solar structure.

*600,917*
**PB87-107090** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Degraded Aqueous Glycol Solutions: pH Values and the Effects of Common Ions on Suppressing pH Decreases.**
Final rept.,
J. R. Clifton, W. J. Rossiter, and P. W. Brown. 1985, 10p
Sponsored by Department of Energy, Washington, DC.
Pub. in Solar Energy Materials 12, n1 p77-86 1985.

Keywords: *pH, *Ethylene glycols, Glycols, Chemical reactions, Reprints, *Solar collectors, *Heat transfer fluids, *Glycol/propylene, *Common ions effect, *Plat plate collectors, Thermal analysis.

Aqueous solutions of ethylene glycol and propylene glycol are used as heat transfer liquids in flat-plate solar collector systems. Both of the glycols are susceptible to thermo-oxidative reactions, which produce organic acids with a resulting decrease in pH of the solutions. The effects of temperature, metals, common ions, and oxidation conditions on the thermal stability of the glycol solutions were evaluated based on measuring changes in pH. Aerated heated glycol solutions produced acidic solutions within 3360 hours (140 days) of testing, when in contact with either metallic aluminum or copper. Common ions (anions of the acid degradation products) were effective in suppressing decreases in pH, especially when aluminum was present.

*600,918*
**PB87-107108** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Evaluation of the Variation in Thermal Performance in a Na2SO4. 10H20 Phase-Change System.**
Final rept.,
P. W. Brown, J. W. Grimes, and L. Kaetzel. 1986, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in Solar Energy Materials 13, n6 p453-461 1986.

Keywords: *Hydrates, *Sodium sulfates, Variations, Phase transformation, Microstructure, Thermodynamic properties, Crystal growth, Solar energy, Reprints.

The relationship between the microstructural changes occurring in a nucleated and thickening Na2SO4-10H2O phase change system, the phase change temperature, and the number of thermal cycles has been investigated. With an increasing number of thermal cycles, the phase change on cooling becomes increasingly athermal in nature. Although this is accompanied by an increase in size of the Na2SO4-10H2O crystals, these variations in phase change temperature appear to be more closely related to the segregation of the nucleating agent.

*600,919*
**PB87-108650** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Life-Cycle Costing of Solar Energy Investments.**
Final rept.,
G. T. Sav, R. T. Ruegg, and J. W. Powell. Jun 81, 8p
Contract DOE-EG-77-C-01-4042
Sponsored by Department of Energy, Washington, DC.
Pub. in Solar Design Workbook, Ch11 p11-1 - 11-8 1981.

Keywords: *Solar energy, *Federal buildings, *Life-cycle cost.

The paper consists of two chapters on solar energy economics prepared for the Solar in Federal Buildings Demonstration Program. The first chapter, 'Life-Cycle Costing of Solar Energy Investments', provides an overview of the life-cycle cost method of evaluating investments in solar energy. Its emphasis is on promoting a general understanding of the approach and is applicable to most solar energy projects. The second chapter, 'Life-Cycle Cost Evaluation of Solar Demonstration Projects', focuses specifically on the application of the life-cycle costing method to projects proposed under the Solar in Federal Buildings Program.

*600,920*
**PB87-109476** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Solar Collector Industry and Solar Energy.**
Final rept.,
W. L. Warnick, and J. E. Hill. Feb 80, 6p
Pub. in Monthly Energy Review, pi-vi Feb 80.

Keywords: Solar energy, Estimating, Economic analysis, Reprints, *Solar industry, *Solar collectors.

From a 1974 level of 1.3 million square feet, the production of solar collectors increased over ten-fold to 13.9 million square feet in 1979 (based upon the first 6-months' data). However, shipments of the various types of collectors, while increasing overall, show sporadic growth patterns over the 5 1/2-year period. Furthermore, a 4-year period of exponential growth appears to have ended.

*600,921*
**PB87-118089** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Design and Evaluation of Thermosiphon Solar Hot Water Heating Systems.**
Final rept.,
J. E. Braun, and A. H. Fanney. 1983, 6p
Sponsored by Department of Energy, Washington, DC.
Pub. in Progress in Solar Energy, v6 p283-288 1984.

Keywords: *Hot water heating, Mathematical models, Reprints, *Thermosiphons, *Solar heating systems, US NBS, TRNSYS computer program.

In the paper, a detailed model for a thermosiphon water heater, to be included in version 12 of the TRNSYS hourly simulation program, is presented. The model utilizes collector parameters determined from standard tests. The component is general for systems with or without in-tank auxiliary heaters. Results of the model compare well with experimental results for both auxiliary energy usage and thermosiphon flow rates and temperatures. TRNSYS is then used to investigate the design and performance of thermosiphon systems for a variety of conditions.

*600,922*
**PB87-119624** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Testing of Refrigerant-Charged Solar Domestic Hot Water-Systems.**
Final rept.,
A. H. Fanney, and C. P. Terlizzi. 1985, 14p
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.
Pub. in Solar Energy 35, n4 p353-366 1985.

Keywords: *Solar heating, *Hot water heating, Refrigerants, Simulation, Tests, Water, Reprints, Hot-water systems.

A repeatable test method independent of outdoor environmental conditions and laboratory geographical location is required in order to provide a means by which solar domestic hot water systems may be rated and compared. The experimental investigation presented in the paper describes two techniques which meet the above criteria for a refrigerant-charged solar domestic hot water system.

# ENVIRONMENTAL POLLUTION & CONTROL

## Air Pollution & Control

*600,923*
**PB86-154598** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Rationale and Plan for Center for Building Technology Research to Improve Indoor Air Quality,**
P. E. McNall. Jan 86, 89p NBSIR-86/3305

Keywords: Air pollution, Measurements, Buildings, *Indoor air pollution, *Air quality.

The report outlines a suggested five year research plan for the Center for Building Technology (CBT) in support of resolving the emerging indoor air quality problem. The problem is defined, and the past research is summarized. The important Federal responsibilities are identified. NBS contributions and capabilities are noted. Future research needs are covered, and these form the basis for the CBT research plan, in cooperation with other Federal agencies, state and local governments, and the private sector.

*600,924*
**PB86-195500** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Smoke Control in VA (Veterans Administration) Hospitals.**
Final rept.,
J. H. Klote. 1985, 4p
Pub. in ASHRAE (American Society of Heating, Refrigeration and Air-Conditioning Engineers) Jnl. 27, n4 p42-45 1985.

Keywords: *Smoke, *Air pollution control, *Air pollution detection, Reprints, *Veterans Administration Hospitals.

The Veterans Administration (VA) has sponsored a project at the Center for Fire Research of the National Bureau of Standards to study smoke control in VA hospitals and to develop new design approaches and methods of acceptance testing. The paper is a report of the ongoing project, and it presents the results of a field test on the San Diego VA Hospital.

*600,925*
**PB86-206364** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.

**Journal of Research of the National Bureau of Standards, Volume 91, Number 1, January-February 1986.**
Feb 86, 44p
See also PB86-206372 through PB86-206414, and PB86-165776. Also available from Supt. of Docs as SN703-027-00008-3.

Keywords: *Acidification, *Mechanical properties, *Precipitation(Meteorology), Durability, Test methods, pH, Raindrops, Chemical analysis, Standards, Mathematical models, Measurement, *Ruggedness, Acid rain.

Ruggedness Testing-Part I: Ignoring Interactions; Ruggedness Testing-Part II: Recognizing Interactions; Effect of Variables on pH Measurement in Acid-Rain-Like Solutions as Determined by Ruggedness Tests; An Interlaboratory Test of pH Measurements in Rainwater; Development of a Standard Reference Material for Rainwater Analysis. The Journal of Research of the National Bureau of Standards features advanes in measurement methodology and analyses consistent with the NBS responsiblity as the nation's measurement science laboratory. It includes reports on instrumentation for making accurate and precise measurements in fields of physical science and engineering, as well as the mathematical models of phenomena which enable the predictive determination of information in regions where measurements may be absent. Papers on critical data, calibration techniques, quality assurance programs, and well characterized reference materials reflect NBS programs in these areas.

*600,926*
**PB86-206398**
(Order as PB86-206364, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Effect of Variables on pH Measurement in Acid-Rain-Like Solutions as Determined by Ruggedness Tests,**
G. Marinenko, R. C. Paule, W. F. Koch, and M. Knoerdel. 4 Nov 85, 6p
Included in Jnl. of Research of the National Bureau of Standards, v91 n1 p17-22 Jan-Feb 86.

Keywords: *Electrodes, *Measurement, *Durability, Glass, pH, Performance evaluation, Calibrating, Tables(Data), *Acid rain.

Ruggedness Test (RT) experiments were performed to assess the significance of the various main factors whiich affect pH measurements in low ionic strength aqueous solutions, as well as to establish the presence of interactions between the main factors. Stirring has an adverse effect on the measurement of pH, since it not only increases the random noise but also biases the measured value. Temperature control to the nearest 0.5 C is sufficient for maintaining measurements accurate to 0.01 pH. Addition of NaNO3 or KC1 can not be tolerated in accurate pH measurements. Three small two-factor interactions were also revealed.

*600,927*
**PB86-206406**
(Order as PB86-206364, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Interlaboratory Test of pH Measurements in Rainwater,**
W. F. Koch, G. Marinenko, and R. C. Paule. 23 Oct 85, 10p
Included in Jnl. of Research of the National Bureau of Standards, v91 n1 p23-32 Jan-Feb 86.

Keywords: *pH, *Acidity, *Rain, Electrodes, Measurement, Reliability, Trends, *Rainwater, *Acid rain.

An interlaboratory test of pH measurements in rainwater has been conducted. Various types of electrodes and junction materials were used in the test. The results of the exercise verify that there are significant differences in the pH values of low ionic strength solutions reported by various laboratories.

*600,928*
**PB86-206414**
(Order as PB86-206364, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Development of a Standard Reference Material for Rainwater Analysis,**
W. F. Koch, G. Marinenko, and R. C. Paule. 9 Oct 85, 9p
Included in Jnl. of Research of the National Bureau of Standards, v91 n1 p33-41 Jan-Feb 86.

Keywords: *Acidity, *Rain, pH, Chemical analysis, Statistical analysis, Standard reference material, Rainwater.

The paper describes the development of Standard Reference Material, SRM 2694, 'Simulated Rainwater,' intended to aid in the analysis of acidic rainfall. Details of the formulation and preparation of the two levels of solutions (2694-I and 2694-II) are given. The 10 analytical techniques used to measure the 12 components in the solutions are described in brief.

*600,929*
**PB86-210556** PC **A06**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Smoke Control at Veterans Administration Hospitals,**
J. H. Klote. Jan 86, 109p NBSIR-85/3297
Sponsored by Veterans Administration, Washington, DC.

Keywords: *Smoke, *Air pollution control, *Air pollution detection, *Veterans administration hospitals.

The Veterans Administration (VA) has sponsored a project at the Center for Fire Research of the National Bureau of Standards to study smoke control in VA hospitals and evaluate design system approaches and methods of acceptance testing. The report presents general background information that is believed to be of interest to those tasked with design, construction and acceptance testing of smoke control systems. The performance requirements of smoke control systems for VA hospitals are discussed. The results of field tests at five VA hospitals is presented and discussed. Based on the information gained from the field tests and the background information, different approaches to smoke control at VA hospitals and methods of acceptance testing are evaluated. General recommendations concerning smoke control at VA hospitals are made.

*600,930*
**PB86-247483** PC **A05**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Methods and Procedures Used at the National Bureau of Standards to Prepare, Analyze and Certify SRM (Standard Reference Material) 2694, Simulated Rainwater, and Recommendations for Use.**
Final rept.,
W. F. Koch. Jul 86, 82p NBS/SP-260/106
Also available from Supt. of Docs as SN003-003-02750-2. Library of Congress catalog card no. 86-600562.

Keywords: *Acidity, *Rain, pH, Chemical analysis, Statistical analysis, Standard reference material, Rainwater.

The report describes the development, preparation, analysis and certification of Standard Reference Material, SRM 2694, Simulated Rain-water, intended to aid in the analysis of acidic rainfall. Details of the formulation and preparation of the two levels of solutions (2694-I and 2694-II) are given, as well as those of the precursor to the SRM, namely Research Material, RM 8409, Simulated Rainwater. The analytical techniques used to measure the twelve components in the solutions are described in detail. The data used in the statistical evaluation of the results are summarized and the recommended values for pH, specific conductance, acidity, fluoride, chloride, nitrate, sulfate, sodium, potassium, ammonium, calcium, and magnesium are tabulated. The instability of ammonium ion in acidic solutions is discussed. Recommendations for the use of SRM 2694, particularly with regard to the measurement of pH, are given.

*600,931*
**PB87-106357** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Atmospheric Carbon: The Importance of AMS (Accelerator Mass Spectrometry).**
Final rept.,
L. A. Currie, G. A. Klouda, and K. J. Voorhees. 1984, 9p
Pub. in Nuclear Instruments and Methods in Physics Research B233, n2 p371-379 1984.

Keywords: *Air pollution, *Aerosols, *Carbon, Carbon 14, Particle size, Sources, Aromatic polycyclic hydrocarbons, Urban areas, Reprints, *Particulate sampling.

Knowledge of the sources, transport and sinks for carbonaceous gases and particles in the atmosphere is of great concern both for understanding the carbon cycle and for assessing man's influence on atmospheric visibility, health effects and climate. Carbon isotopes (notably (14)C) are extremely important in tracing such species and in validating models based on emissions inventories, dispersion algorithms, and trace inorganic or organic mass balance. Accelerator Mass Spectrometry (AMS) offers tremendous promise to this field, for useful sample size may be decreased by three orders magnitude, resulting in greatly improved spatial, temporal and chemical resolution. Special problems which have been attacked with the help of (14)C-AMS are reviewed, including the study of sources of elemental, organic (particulate), and gaseous carbon compounds in the atmosphere. The report concludes with a brief review of techniques which have been used for 10-100 micrometers carbon samples, and a discussion of special atmospheric (Urban Particulate) Standard Reference Materials.

*600,932*
**PB87-116224** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Atmospheric Deposition Reference Materials: Measurement of pH and Acidity.**
Final rept.
W. F. Koch, and G. Marinenko. 1983, 12p
Sponsored by Air Pollution Control Association, Pittsburgh, PA.
Pub. in Proceedings of Annual Meeting on Air Pollution Control Association (76th), Atlanta, GA., June 19-24, 1983, v3 12p.

Keywords: *pH, *Acidity, *Air pollution control, Chemical analysis, Atmospheric composition, Environments, Trace elements, *Acid rain, *Reference materials, Precipitation washout, Standard reference materials.

The Center for Analytical Chemistry of the National Bureau of Standards has the mandated responsibility to the nation for maintaining the quality assurance of chemical measurements. In the area of atmospheric deposition, this role includes methods development research, as well as analysis and issuance of standards. The measurement of pH in solutions of low ionic strength is being studied with an effort toward improving the precision, accuracy, and thermodynamic significance of the measured value. The determination of total acidity in rainfall is also being investigated with the focus on the reduction of errors associated with titrations of low levels of acid and endpoint location. Several Standard Reference Materials are currently available which have direct applicability to air-particulate, gas, and water analyses. In a cooperative effort with the Environmental Protection Agency, several sets of simulated precipitation reference materials have been produced and analyzed to be used as a means of intercalibrating atmospheric monitoring stations. Additional research is required to improve measurement protocols and to establish the standards needed to assure measurement comparability and consistency throughout the nation.

## Noise Pollution & Control

*600,933*
**PB86-166188** PC **A12**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Guidelines for the Prevention of Traffic Noise Problems,**
F. F. Rudder, and S. L. Yaniv. Jan 86, 264p NBSIR-86/3311/DOT
Contract DTFH61-83-Y-10014
Sponsored by Federal Highway Administration, McLean, VA. Office of Implementation.

Keywords: Noise reduction, Transportation, Land use, Guidelines, *Traffic noise.

The guidelines describe a consistent methodology for the identification and prevention of traffic noise problems by emphasizing noise-compatible land development. The guidelines are a self-contained document. The methodology provides for the quantitative evaluation of both the severity of traffic noise problems and the mitigation of these problems. Although calculations are required, specialized training in acoustics or

noise control is not necessary to utilize the methodology. Methods are provided for prediction of highway traffic, diesel-electric railway, and existing levels of environmental noise. These levels serve to identify the severity of the noise problem. Mitigation techniques are presented that may be utilized to reduce or eliminate traffic noise problems.

## Radiation Pollution & Control

*600,934*
**PB86-193091** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Determination of Iodine-129 at Natural Levels by Thermal Neutron Activation Analysis.**
Final rept.,
G. J. Lutz, H. L. Rook, and R. M. Lindstrom. 1984, 19p
Pub. in Jnl. of Trace Microprobe Tech. 2, n1 p33-51 1984.

Keywords: *Radioactive contaminants, *Radioactivation analysis, Reprints, *Iodine 129, *Activation analysis.

(129)I is a long-lived fission product (half-life = 15,900,000 years) produced from natural sources as well as from nuclear reactors and nuclear explosions. Neutron activation analysis is a very sensitive method for determining (129)I. A limiting factor of sensitivity is the decontamination of the product nuclide (130)I from (82)Br. The selective ion retention medium, hydrated manganese dioxide, is shown to be effective in achieving the separation. Decontamination of the order of 1,000,000 from (82)Br with a 90% yield of (130)I is realizable.

## Solid Wastes Pollution & Control

*600,935*
**AD-A139 213/3** PC **A06**/MF **A01**
National Bureau of Standards (NML), Washington, DC. Chemical Kinetics Div.
**Combustion Technology for Incinerating Wastes from Air Force Industrial Processes.**
Final rept. Jun 81-Jun 83,
W. M. Shaub, and W. Tsang. Feb 84, 121p AFESC/ESL-TR-83-14
Contract MIPR-N-8146

Keywords: *Waste disposal, *Waste management, Air Force facilities, Solid wastes, Hazardous materials, Combustion, Incinerators, Air pollution, Heat, Recovery, Utilization, *Incineration, Waste utilization.

Air Force bases, particularly Air Logistics Centers, generate significant amounts of process wastes from a variety of industrial operations. Some of these wastes are classified hazardous under the Resource Conservation and Recovery Act and are properly disposed at cost to the Air Force. Onsite incineration with heat recovery is being considered as a disposal option, to reduce the overall disposal costs. Since relatively small amounts of single wastes are generated at any one base, an incineration system must be flexible to handle a wide variety of materials. Results indicate a technical basis for using Air Force industrial wastes as supplemental fuels. Suggestions made in this report should enable Air Force personnel to design and execute programs to destroy such wastes, recover energy, and show empirically that applicable environmental laws and regulations have been properly taken into account. Furthermore, a technique to allow decision makers to select least-cost options to use the suggestions made in this report exists, i.e., a modified form of the resource recovery planning model (RRPLAN) developed at the National Bureau of Standards.

## Water Pollution & Control

*600,936*
**PB87-107124** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Biological Mediation of Marine Metal Cycles: The Case of Methyl Iodide.**
Final rept.,
F. E. Brinckman, G. J. Olson, and J. S. Thayer. 1985, 12p
Pub. in Marine Estauarine Geochemistry, p227-238 1985.

Keywords: *Water pollution, Sulfur inorganic compounds, Tin organic compounds, Metals, Transformations, Marine microorganisms, *Marine metal cycling, *Methyl iodide, Heavy metals.

Exocellular biogenic metabolites solubilize and methylate heavy metals and may be important in global metal cycling. The authors found that methyl iodide, ubiquitous in marine environments, though its biogenesis is poorly understood, solubilizes bulk metals and refractory binary and ternary metal sulfides, possibly represented by oceanic suspended particulates, producing methylated sulfur coproducts. With tin, among those elements forming water stable methyl derivatives, the authors report that stannous sulfide and chloride react with MeI to produce methyltin(IV) species and tin(IV) as cassiterite, a major tin ore ($SnO_2$), is solubilized but not methylated by MeI. The authors find that dimethylpropiothetin, a common algal metabolite, reacts with cell-permeable I(1-) to produce MeI and with OH(1-) to form Me2S. Based on these results, the authors construct a model for environmental heterogeneous methylation reactions mediated by intracellular or extracellular MeI and methylsulfonium compounds which may bear on the frequency reported methylmetal(loid) species reported in marine environments.

## General

*600,937*
**PB86-186707** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.
**Environmental Measurements, Standards, and Decisions.**
Final rept.,
W. H. Kirchoff. 1984, 6p
Pub. in AIChE (American Institute of Chemical Engineers) Symposium Series 80, n237 p6-11 1984.

Keywords: *Environments, Measurement, Standards, Regulations, Reprints, American Society for Testing and Materials, Uncertainty.

A pervasive and often ignored condition in the development and implementation of environmental policy is uncertainty. The paper will describe limitations of the measurement system, the role of standards in compensating for uncertainty, and features of the American Society for Testing and Materials, ASTM, and its process for setting standards which offer alternatives to litigation and confrontation as approaches to reaching consensus.

*600,938*
**PB86-204005** PC **A05**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD.
**Summary of the Environmental Research, Analysis, and Control Standards Issued by the National Bureau of Standards.**
Final rept.,
R. Mavrodineanu, and S. D. Rasberry. Mar 86, 95p NBS/SP-260/105
Also available from Supt. of Docs as SN003-003-02725-1. Library of Congress catalog card no. 86-600504.

Keywords: *Chemical composition, *Chemical analysis, Standards, Measurement, Quality control, Tables(Data), *Environmental research, *Standard reference materials, National Bureau of Standards.

The publication is a summary of the environmental research, analysis, and control standards issued by NBS as Standard Reference Materials (SRM's). The material, composition, certification, use, and remarks concerning each of the SRM's described are presented in tabular form. Copies of the certificates of these SRM's are contained in the appendix for more detailed information.

*600,939*
**PB87-131421** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Resistance to Standards Development.**
Final rept.,
W. H. Kirchhoff. 1984, 3p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 12, n6 p21-23 1984.

Keywords: *Standards, Resistance, Reprints, *Environmental assessment, American Society for Testing and Materials.

In the recent years, the American Society for Testing and Materials, ASTM, has experienced rapid growth in standards writing activities related to environmental assessment. The growth has brought into the membership of ASTM individuals from scientific disciplines new to ASTM and for whom ASTM was a strange and confusing society. Not surprisingly, many of these individuals initially resisted ASTM incursion into their field. The causes of the resistance have been interesting and have provided both guidance for approaching individuals from new disciplines and insight into the social dynamics of standards development. The paper will review the author's experience in dealing with the expansion of ASTM activities into environmental assessment.

# HEALTH CARE

## Health-Related Costs

*600,940*
**PB87-117933** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
**Assessing the Costs of Fire Protection in Health Care Facilities.**
Final rept.,
R. E. Chapman. 1985, 11p
Pub. in Fire Safety Jnl. 9, n2 p221-231 Jul 85.

Keywords: *Fire protection, *Health facilities, *Cost estimates, Reprints.

The identification of cost-effective levels of fire safety in health care facilities is a major concern to hospital administrators, fire safety engineers, and public policymakers. Rising construction and operating costs coupled with more stringent building codes and continuing advances in medical and building technology have complicated the issue, forcing health care facility administrators to assess carefully the alternative means through which they can design, construct, or update their facilities. The paper illustrates how the use of a performance-based approach to fire safety can dramatically reduce the costs of code compliance without reducing the safety and well-being of those housed in health care facilities.

# INDUSTRIAL & MECHANICAL ENGINEERING

## Environmental Engineering

*600,941*
**PB86-193059** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

## Environmental Engineering

**Indoor Humidity Calculations.**
Final rept.,
T. Kusuda. 1983, 1p
Pub. in ASHRAE (American Society of Heating, Refrigeration and Air-Conditioning Engineers) Jnl. 25, n5 p64 1983.

Keywords: *Humidity, Humidity control, Computation, Dew point, Absorption, Desorption, Reprints.

Measured hourly data on indoor humidity is compared with the data obtained by the calculated values for NBS Houston test houses and for the high mass test building in an environmental chamber. The paper also introduced the Tsuchiya model that permits the evaluation of room surface moisture absorption capability. The model is based upon the detailed simulation calculation for the room moisture balance that includes the surface condensation evaporation and absorption/desorption coefficients. These coefficients were determined in such a manner that the measured room humidity levels coincide with the calculated values.

## Industrial Safety Engineering

*600,942*
**PB86-162153** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Ceiling Jet Properties and Wall Heat Transfer in Compartment Fires near Regions of Ceiling Jet-Wall Impingement,**
L. Y. Cooper. Jan 86, 34p NBSIR-86/3307

Keywords: *Ceilings(Architecture), *Fires, Heat transfer, *Compartment fires, Fire models.

The problem of heat transfer to walls from fire plume-driven ceiling jets during compartment fires is introduced. An analogy is drawn between the flow dynamics and heat transfer at ceiling jet-wall impingement and at the line impingement of a wall and a two-dimensional, plane, free jet. Using the analogy, the literature on plane, free jet flows and corresponding wall stagnation heat transfer rates leads to readily useable estimates for the heat transfer from, and the mass, momentum, and enthalpy fluxes of the turned compartment fire ceiling jet as it begins its initial descent as a negatively buoyant flow along the compartment walls. Available data from a reduced-scale experiment provides some limited verification of the heat transfer estimate.

*600,943*
**PB86-177722** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Basic Structure of the Fire Protection Design Assessment System,**
H. E. Nelson, and W. D. Walton. Feb 86, 30p NBSIR-85/3298
Sponsored by Air Force Engineering and Services Center, Tyndall AFB, FL.

Keywords: *Fire protection, Systems engineering, Safety engineering, Smoke, Buildings, Fires, Compartment fires, Fire studies.

The purpose of the Fire Protection Design Assessment System is to provide design engineers with a tool to improve their ability to appraise the overall fire safety in a facility and evaluate the impact of fire protection measures. The system is based on deterministic fire prediction techniques and will be implemented through an interactive computer program. The report describes the components and basic structure of the system. The inputs to system include data on the building layout, combustible contents, fire resistance, detectors, sprinklers, smoke control system, occupants and the fire safety objectives. The outputs include the predicted fire generated conditions within the building as a function of time and an evaluation of the user specified fire safety objectives.

*600,944*
**PB86-181849** PC **A03**/MF **A01**
California Univ., Berkeley. Dept. of Mechanical Engineering.
**Fire Propagation in Concurrent Flows. Final Progress Report June 1, 1984-May 31, 1985,**
A. C. Fernandez-Pello. Feb 86, 50p NBS/GCR-86/505
Grant NB83-NADA-4020
See also PB85-101129. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Flame propagation, *Fire tests, Flames, Flow, Heat transfer, Combustion.

A study is currently underway of the spread of flames over the surface of a solid combustion of a solid combustible in a mixed, forced and free, convective flow. Research efforts have concentrated primarily on a experimental study of the flow assisted spread of flames over thermally thin fuels, and a numerical analysis of the extinction of flames established over a flat combustible surface. The experimental results indicate that wind aided fire spread is primarily controlled by heat transfer from the flame to the unburnt combustible. The flame spread rate data can be correlated with and expression obtained from a heat transfer analysis of the flame spread process.

*600,945*
**PB86-182292** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**ASKBUDJr: A Primitive Expert System for the Evaluation of the Fire Hazard of a Room,**
R. L. Smith. Mar 86, 65p NBSIR-86/3319

Keywords: *Fire safety, Artificial intelligence, Computer programs, Fire hazards.

The Center for Fire Research (CFR) has a long-term project to develop expert systems as a technology transfer mechanism. CFR has as the long-term goal of the project: to develop a computer program which will make an expert estimate of the fire safety of a building based on CFR's deterministic physical models, technical data, and the expert judgement of its staff.

*600,946*
**PB86-185246** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Toxic Hazard Evaluation of Plenum Cables.**
Final rept.,
R. W. Bukowski. Nov 85, 15p
Pub. in Fire Technology 21, n4 p252-266 Nov 85.

Keywords: *Toxicity, *Power lines, *Fire hazards, Electrical insulation, Reprints.

Code provisions covering the installation of low voltage cables in plenum spaces above suspended ceilings used for environmental air are reviewed. A calculation procedure which could be used to estimate the potential toxicity of the decomposition products from these cables relative to the toxicity of the compartment fire necessary to decompose the cable insulation is presented. These estimates are used in a four-step procedure for estimating Smoke Toxicity Hazard proposed by the NFPA Toxicity Advisory Committee which is described. Example calculations for some typical cases and a discussion of their limitations are included.

*600,947*
**PB86-189743** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**Finite Difference Calculations of Buoyant Convection in an Enclosure: Verification of the Nonlinear Algorithm.**
Final rept.,
R. G. Rehm, P. D. Barnett, H. R. Baum, and D. M. Corley. 1985, 15p
Pub. in Applied Numerical Mathematics 1, p515-529 1985.

Keywords: *Finite difference theory, *Buoyancy, *Convection, Fires, Enclosures, Reprints, Fire studies.

Solutions are presented to nonlinear finite difference equations used to represent fire-driven buoyant convection in enclosures. The solutions depend upon the fact that these difference equations permit the decomposition of the discretized velocity field into solenoidad and irrotational components. The irrotational field is shown to satisfy a finite difference analog of Bernoulli's equation when the density is constant. This leads to a three-dimensional time-dependent solution to the difference equations. The solenoidal field is shown to possess steady-state two-dimensional solutions corresponding to a constant non-zero value of the discretized vorticity. The two solutions, together with results presented elsewhere describing finite difference approximations to linear internal waves in enclosures, have been used in the development and testing of the computer-based algorithms used to solve these equations.

*600,948*
**PB86-192390** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Significance of a Wall Effect in Enclosures with Growing Fires, 1984.**
Final rept.,
L. Y. Cooper. 1984, 21p
See also PB83-235671. Sponsored by Department of Health and Human Services, Washington, DC., and Department of the Interior, Washington, DC.
Pub. in Combustion Science and Technology 40, p19-39 1984.

Keywords: *Buildings, *Fires, Flame propagation, Reprints, *Compartment fires, Fire studies, Room fires, Wall flow.

The paper studies the significance of a wall effect that has been observed during the growth stage of enclosure fires. Relative to the two-layer phenomenon which tends to develop during such fires, the effect has to do with the near-wall downward injection of hot upper layer gases into the relatively cool uncontaminated lower layer. It is conjectured that these observed wall flows are buoyancy driven, and that they develop because of the relatively cool temperatures of the upper wall whose surfaces are in contact with the hot upper layer gases. The results of the analysis indicate the importance of taking the wall effect into account in two-layer zonal analyses of enclosure fire phenomena.

*600,949*
**PB86-196417** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Salt Water Modeling of Fire Induced Flows in Multicompartment Enclosures,**
K. D. Steckler, H. R. Baum, and J. G. Quintiere. Mar 86, 53p NBSIR-86/3327
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.

Keywords: *Fires, *Model tests, Flow visualization, Salt water, Smoke, Buoyancy, Enclosures, *Fire models, Compartment fires.

Salt water modeling is used to study fire-induced flows in multicompartment structures. Scaling laws relating salt water flows and hot gas flows are developed. Results from 1/20 scale salt water simulations of fire-induced flows in a single-story multiroom structure are shown to be in good agreement with available full-scale results. Experiments involving a 1/20 scale model of a U.S. Navy ship demonstrate the feasibility of using the technique to study hot gas flows in compartmented structures too complex to study economically by other means.

*600,950*
**PB86-203817** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Fire Research Publications, 1985,**
N. H. Jason. May 86, 46p NBSIR-86/3372
See also PB85-208502.

Keywords: *Fires, Fire safety, Smoke, Toxicity, Fire protection, *Fire studies, Compartment fires, Fire models.

'Fire Research Publications, 1985' is a supplement to previous editions: Earlier editions, i.e., 1969-1979, also are available in the National Technical Information Service (NTIS). Only publications prepared by members of the Center for Fire Research (CFR), by other National Bureau of Standards (NBS) personnel for CFR, or by external laboratories under contract or grant from the CFR are cited.

*600,951*
**PB86-206570** PC **A24**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

**Evaluating Thermal Fire Detection Systems (English Units).**
Final rept.,
D. W. Stroup, D. D. Evans, and P. Martin. Apr 86, 559p NBS/SP-712
Also available from Supt. of Docs as SN003-003-02727-8. Library of Congress catalog card no. 86-600519

Keywords: *Fire detection systems, *Buildings, Fire damage, Fire protection, Fire resistance, Data, Computer programs, Computer applications.

The report presents a methodology for evaluating heat detection systems installed in buildings. Previous work for use primarily in designing new thermal fire detection systems was used as a starting point. The previous work was enhanced and supplemented to make it more useful for evaluating existing systems. The resulting equations were programmed into a user interactive computer program. The program is available in both BASIC and FORTRAN and will run on mainframes as well as personal computers. In addition, a modified version of the FORTRAN program was used to develop an extensive set of tables listing detector activation times for given building geometries, detector characteristics, and fire growth rates. These tables are useful for quick evaluation of alternative heat detector installations. Finally, practical examples are included to illustrate the use of the tables and computer programs.

*600,952*
**PB86-210002** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Use of Fire Statistics in Assessing the Fire Risk of Products.**
Final rept.,
D. Gross. 1985, 8p
Pub. in Proceedings of International Conference on Flammability, INTERFLAM '85 Conference Workbook, Guildford (England, March 26-28, 1985, p22-18.

Keywords: *Statistical analysis, *Curtains, Fire tests, Fire hazards, Risk, Fire losses.

In assessing the fire risk of one or more specific products, fire incidence statistics provide an important base line measure of the extent of fire losses, and of the principal causative factors, including sources of ignition and the effects of occupancy and fire protective measures. Normalizing the incidence data in terms of the exposure time, the available exposed area of the product, and the number of persons at risk may permit more meaningful comparisons to be made. Analysis of the likely fire scenarios leading from ignition to an ultimate injury or loss provides insight into the fire response factors important in laboratory evaluation of a product.

*600,953*
**PB86-212073** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Perimeter Safety Net Projection Requirements,**
C. W. C. Yancey, N. J. Carino, and M. Sansalone. May 86, 61p NBSIR-85/3271
Sponsored by Occupational Safety and Health Administration, Washington, DC.

Keywords: *Construction, *Nets, *Safety engineering, Requirements, Regulations, Tests, Mathematical models, Guidelines, Falling bodies, *Occupational safety and health.

Current construction-site safety net regulations set limitations on the minimum horizontal projection of perimeter nets and the maximum vertical distance between an elevated working surface and the net below. These limitations were arbitrarily established as no actual or simulated fall data existed. The adequacy of these requirements in ensuring construction worker safety has been questioned. Thus, a test program was carried out to determine the adequacy of existing regulations. Simulated fall tests were conducted using anthropomorphic dummies to represent falling workers. Results are presented to show the trajectory of the falling body and the maximum horizontal distance in the final landing position. An analytical model was developed to simulate a falling worker. The model can be used to predict trajectories for a given set of initial conditions including worker height and weight, departure horizontal velocity and fall height. Guidelines are presented for revising existing regulations pertaining to the dimensional requirements for perimeter nets.

*600,954*
**PB86-226594** PC **A10**/MF **A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Examination of a Pressure Vessel that Ruptured at the Chicago Refinery of the Union Oil Company on July 23, 1984,**
H. I. McHenry, T. R. Shives, D. T. Read, J. D. McColskey, and C. H. Brady. Mar 86, 205p NBSIR-86/3049
Sponsored by Occupational Safety and Health Administration, Washington, DC.

Keywords: *Pressure vessels, Brusting, Examination, Corrosion, Hydrogen embrittlement, Fracture(Mechanics).

The pressure vessel fractured along a path that was weakened by extensive cracking adjacent to a repair weld joining a replacement section to the vessel. These pre-existing cracks initiated in areas of a hard microstructure known to be susceptible to hydrogen stress cracking. The microstructure formed during the repair welding of the replacement section, and at the surface, it was not tempered by subsequent weld passes or thermal treatment. The cracks grew through the vessel wall due to hydrogen pressure cracking. When the depth of the largest of these pre-existing cracks exceeded 90 to 95% of the wall thickness, leakage occurred because the thin ligament of steel remaining in the cracked section ruptured. Because of the uniform depth of the pre-existing crack, the thin ligament continued to tear, causing the through crack to grow to a length of about 800 mm. The crack triggered final fracture at the operating stress level of 35 MPa because the toughness of the vessel steel was reduced by hydrogen embrittlement.

*600,955*
**PB86-230471** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Concepts for Life Safety Analysis.**
Final rept.,
H. E. Nelson. 1986, 19p
Pub. in Proceedings of Society of Fire Protection Engineers Symposium on Quantitative Methods for Life Safety Analysis (7th), College Park, MD., March 5-7, 1986, p1-19.

Keywords: *Fire protection, *Fire hazards, Fire safety, Smoke, Fire detection systems, Fire models, Fire studies.

An overview of the need, methods, and resources appropriate for life safety analysis of fire hazard is presented. An outline of the elements of a fire hazard analysis system with appropriate references is given.

*600,956*
**PB86-230810** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Measure of Evacuation Difficulty.**
Final rept.,
B. M. Levin, H. E. Nelson, and N. E. Groner. 1982, 9p
Pub. in Proceedings of International Fire Protection Seminars (6th), Karlsruhe, Germany, September 21-24, 1982, p323-331.

Keywords: *Fire safety, *Fire protection, *Evacuating(Transportation), Building codes, Fire detection systems.

Fire safety requirements are being developed for buildings housing disabled people including the mentally retarded. Some disabled people can escape a building rapidly without assistance while others need someone to help them. More fire protection features need to be built into the building when the disabled residents require assistance to evacuate. A procedure has been developed to evaluate or measure the difficulty of evacuating residences housing disabled people. The measure is used to determine the fire protection features to be built into the building; the greater the evacuation difficulty, the more fire protection features required.

*600,957*
**PB86-230828** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Progress Report on Fire Investigation.**
Final rept.,
A. Gomberg. 1982, 8p
Pub. in Proceedings of Joint Panel Meeting UJNR Panel on Fire Research and Safety (6th), Tokyo, Japan, May 10-14, 1982, p39-46.

Keywords: *Fires, *Fire investigation, Fire reporting, Fire studies.

Progress made on several fronts in the area of fire investigation in the U.S. in recent years is discussed. Improvements in both the quantity and quality of U.S. Fire Investigations is referenced, including fire reporting, post fire interviews and special studies.

*600,958*
**PB86-232428** PC **A24**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Evaluating Thermal Fire Detection Systems (SI Units).**
Final rept.,
D. W. Stroup, D. D. Evans, and P. Martin. Apr 86, 560p NBS/SP-713
See also PB86-206570. Library of Congress catalog card no. 86-600520.

Keywords: *Fire detection systems, *Buildings, Fire damage, Fire protection, Fire resistance, Sprinkler systems, Fire safety, Fire alarm systems.

The report presents a methodology for evaluating heat detection systems installed in buildings. Previous work for use primarily in designing new thermal fire detection systems was used as a starting point. The previous work was enhanced and supplemented to make it more useful for evaluating existing systems.

*600,959*
**PB86-232691** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**ASET - A Computer Program for Calculating Available Safe Egress Time.**
Final rept.,
L. Y. Cooper, and D. W. Stroup. 1985, 17p
Pub. in Fire Safety Jnl. 9, p29-45 1985.

Keywords: *Fire tests, Combustion products, Smoke, Reprints, *Fire studies, Compartment fires, Fire investigation, Room fires.

A user-oriented computer program which carries out the required simulations and provides estimates for the ASET has been developed. Describes the program and its use. For fire growth in a particular fuel assembly, a single program run can be used to evaluate the ASET from enclosures (which are assumed to contain the fuel assembly) of different heights and areas, and under a variety of different detection and hazard criteria.

*600,960*
**PB86-240066** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Pillow Burning Rates.**
Final rept.,
V. Babrauskas. 1985, 2p
Pub. in Fire Safety Jnl. 8, n3 p199-200 1985.

Keywords: *Fire tests, *Burning rate, Fire safety, Combustion, Fire resistance, Reprints, *Fire studies, *Pillow.

Burning rates have been determined for four common pillow types and one of newer design, intended to be especially fire resistive. One replicate test was run and showed satisfactory reproducibility. The order of performance, best to worst, was: fiberfill (protected with fiberglass cover); feathers; fiberfill (ordinary construction); polyurethane foam; latex foam.

*600,961*
**PB86-240082** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Some Characteristics of Fabrics for Heat Protective Garments.**
Final rept.,
J. F. Krasny. 1986, 12p
Pub. in ASTM (American Society for Testing and Materials) STP 900, p463-474 1986.

## Industrial Safety Engineering

Keywords: *Protective clothing, Fire resistant textiles, Fire protection, Clothing, Reprints, Fire fighters.

Principles of protection afforded by clothing in fire situations are reviewed briefly. Several examples of measurements of heat protective properties are given. Materials covered are single layers of fabrics appropriate for work uniforms, the same type of fabric combined with four popular underwear fabrics, and typical fire fighters' turnout coat assemblies, consisting of a shell fabric, vapor barrier, and thermal barrier.

*600,962*
**PB87-100996** PC **A09**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**User's Guide for RAPID, Reduction Algorithms for the Presentation of Incremental Fire Data.**
Final rept.,
J. N. Breese, and R. D. Peacock. Aug 86, 199p
NBS/SP-722
Also available from Supt. of Docs as SN003-003-02752-9. Library of Congress catalog card no. 86-600565.

Keywords: *Fire tests, Algorithms, Computer systems programs, Computer programs, Data.

RAPID is a stand-alone program specifically designed to convert raw instrument voltages collected during such tests into meaningful units. The reduced data can also be used alone or in combinations to obtain quantities that require more than minimal data reduction.

*600,963*
**PB87-105201** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**National Bureau of Standards Conference on Fire Research, 1981.**
Final rept.,
D. Gross. 1981, 2p
Pub. in Fire and Materials 5, n4 p180-181 1981.

Keywords: *Fire tests, Meetings, Soot, *Fire studies, Fire models.

The Fifth Annual Conference on Fire Research was held at the National Bureau of Standards on August 19-21, 1981. Sponsored by the NBS Center for Fire Research, this Conference permitted 25 CFR grantees from universities and research institutes to present short summaries of progress on their research activities on the more basic aspects of fire research.

*600,964*
**PB87-107926** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Fire Safety.**
Final rept.,
B. Levin, R. Paulsen, and J. Klote. 1981, 8p
Pub. in Access Information Bulletin, p1-8 1981.

Keywords: *Fire safety, Buildings, Reprints, *Handicapped persons, Group homes.

The bulletin discusses two recent trends which have implications for fire safety: the movement of disabled persons from institutional to community settings, and the provision of increased accessibility to public buildings for disabled persons. The bulletin also presents some general principles which should guide emergency planners, and describes some specific hardware devices and systems to assist disabled persons in a fire emergency. It is emphasized that fire safety for disabled persons is a many-faceted problem.

*600,965*
**PB87-107934** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Overview of Fire Modeling.**
Final rept.,
J. G. Quintiere. 1981, 22p
Pub. in SFPE Symposium 'Systems Applications for Fire Protection Engineers', College Park, MD., March 4-6, 1981, p1-22 1981.

Keywords: *Fire tests, *Fire models, Room fires, Fire studies.

A perspective on modeling fire is presented. The evolution of the use of a two-layer zone model to describe the developing fire in a room is traced. Some examples are given to illustrate the results from this type of model. Future implications are discussed.

*600,966*
**PB87-109450** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**How Fire Research Programs are Formulated.**
Final rept.,
J. E. Snell. 1984, 13p
Grants NSF-CEE82-06605, NEA-32-4253-60074
Sponsored by National Science Foundation, Washington, DC., National Endowment for the Arts, Washington, DC., and Federal Emergency Management Agency, Washington, DC.
Pub. in Communications between the Fire Research Community and the Owner-Operators of Buildings--Proceedings Conference, Washington, DC., November 9-10, 1983, p31-43 1984.

Keywords: *Fire protection, Fire tests, Housing, Research management, Reprints.

The CFR research program is designed to provide powerful new capabilities for reducing fire losses and the costs of fire protection. It is based on an analysis of our own capabilities and a complex array of factors in the environment external to the Center for Fire Research. It represents a significant departure from the more conservative course of incremental improvement in those traditional practices for fire protection which have no basis in scientific fact. The course raises a number of issues. Four have been singled out: the need for a viable community of private and public sector researchers; departure from dependence on traditional practices; the need for new institutional mechanisms; and a directed assault on the toughest area of fire loss, in particular, existing residential occupancies. This is clearly not the most expedient nor the easiest course for us to follow. However, it is the one the Congress assigned us nearly a decade ago. Experience today affirms it remains the right one.

*600,967*
**PB87-109468** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Transient Cooling of a Hot Surface by Droplet Evaporation.**
Final rept.,
A. K. Trehan, M. di Marzo, and D. D. Evans. 1985, 4p
Pub. in Proceedings of Fall Technical Meeting Chemical and Physical Processes in Combustion, Philadelphia, PA., November 4-6, 1985, p61-1-61-4.

Keywords: *Extinguishing, *Evaporative cooling, Aluminum, Drops(Liquids), Fire safety, Reprints.

The thermal behavior of a hot surface subjected to a cold liquid droplet impingement and evaporation was investigated using a heated aluminum block, and deionized and degasified water. Evaporation times and droplet radius on the aluminum surface were measured. A thermal conduction model for the cooling of the aluminum was coded to determine radial and in-depth transient temperatures in the area of the evaporating droplet.

*600,968*
**PB87-119822** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Role of ASTM (American Society for Testing and Materials) in Fire Modeling.**
Final rept.,
A. J. Fowell. 1986, 3p
Pub. in American Society for Testing and Materials Standardization News 14, n9 p38-40 Sep 86.

Keywords: *Fire safety, *Mathematical models, Combustion, Heat transfer, Fluid flow, Reprints.

Recent rapid advances in the development of fire modeling techniques and recognition of their potential uses in fire safety have suggested a role for ASTM. The mathematical representation of the fire growth process and its effect on materials and people according to the appropriate mass and energy relationships of combustion, heat transfer, and fluid flow is fire modeling. The following examines the history and current direction of ASTM's role in fire modeling.

*600,969*
**PB87-134730** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Cone Calorimeter: A Versatile Bench-Scale Tool for the Evaluation of Fire Properties.**
Final rept.,
V. Babrauskas. 1986, 10p
Pub. in New Technology to Reduce Fire Losses and Costs, p78-87 1986.

Keywords: *Calorimeters, *Fire detectors, Heat measurement, Ignition, Fire tests, Reprints, Toxic gas production.

The rate of heat release is probably the single most important measure of fire hazard. For fire testing purposes, the scale required even for bench-scale tests is large enough to have precluded affordable, yet competent calorimeters, having small, well-characterized errors. The application of the oxygen consumption principle has now permitted a new generation of heat release measurement apparatuses to be developed for fire testing purposes. The Cone Calorimeter was also seen as a suitable combustor to be used in making other fire hazard measurements. Thus, techniques have been developed for making measurements of ignitability, smoke obscuration, soot production, and the generation of toxic gas species. The promise is also held forth that properties descriptive of flame spread behavior may be simultaneously obtained.

*600,970*
**PB87-145421** PC **A07**/MF **A01**
Maryland Univ., College Park. Dept. of Mechanical Engineering.
**Transient Cooling of a Hot Surface by Droplets Evaporation. Final Report.,**
M. di Marzo, and A. K. Trehan. Jul 86, 133p REPT-86-7, NBS/GCR-86/516
Grant NANB-5-H0525
See also PB87-109468. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Extinguishing, *Evaporative cooling, Aluminum, Drops(Liquids), Fire safety, Computerized simulation, Metal plates.

The thermal behavior of a hot aluminum surface subjected to cold water droplet impingement is investigated. Evaporation phenomena of a single droplet of pure water is studied for initial surface temperature ranging from 75 to 100 deg C (implying full suppression of nucleate boiling). The effect of droplet release height, initial surface temperature and, droplet volume on the geometrical configuration of the droplet is investigated. A computer model is developed to predict the cooling effect (volume of influence) induced by a single droplet in contact with the hot surface, using finite difference techniques. A model to predict the evaporation of water droplets deposited on a hot non-porous solid surface is derived. The water-vapor molar fraction in the air at the exposed surface of the water droplet is deduced from the coupled heat and mass transfer energy balance. Spacial and temporal integration of the overall droplet energy equation is used to predict the droplet evaporation time and the instantaneous evaporation rate. Model predictions agree well with experiments. The model is used to quantify spatial and temporal heat fluxes distribution at the exposed surface of the water droplet. The volume of influence is found to correlate linearly with the evaporation time. This funding is particular important in light of the modelling of multi-droplets cooling effect.

## Laboratory & Test Facilities

*600,971*
**PB87-107082** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Coming Redefinition of Photometry.**
Final rept.,
G. L. Howett. 1986, 14p
Contract DE-AC03-76SF00098
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of the Illuminating Engineering Society 15, n2 p5-18 1986.

Keywords: *Photometry, Luminance, Brightness, Color, Reprints.

The paper is a relatively nontechnical tutorial explanation of the fundamental change in the definition of photometry that appears to be in the offing. The current definition of photometry is reviewed, and the problems with the definition are indicated, including the practical implications of the discrepancy between measured luminance and perceived brightness. The current theoretical explanation of these problems, based on the opponent-colors model, is summarized. The work of the CIE in the area is reviewed and the probable form of a new supplementary definition of photometry and of new photometric instruments is outlined. In order to facilitate coordination among visual scientists publishing in the field, new proposals concerning terminology and notation are offered. The relationship of current theory and data to 'visual sensitivity curves' is described.

*600,972*
**PB87-107140** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Viscometer for Low Frequency, Low Shear Rate Measurements.**
Final rept.,
R. F. Berg, and M. R. Moldover. Aug 86, 6p
Contract NASA-C-86129-D
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Review of Scientific Instruments 57, n8 p1667-1672 Aug 86.

Keywords: *Viscometers, Shear rate, Measurement, Reprints.

The authors describe a torsion-oscillator viscometer whose low frequency (0.5 Hz) and very low shear rate (0.05/s) are required for measurements of shear sensitive fluids such as microemulsions, polymer melts and solutions gels, and liquid mixtures near critical points. The viscometer has a resolution of 0.2% when used with liquid samples and a resolution of 0.4% when used with a dense gaseous sample. The viscometer operates under computer control and is compatible with submillikelvin temperature control.

*600,973*
**PB87-107165** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Miniature Contact Thermometer for Student Use.**
Final rept.,
T. J. Bruno, and J. G. Shepherd. 1986, 1p
Sponsored by Gas Research Inst., Chicago, IL., and Department of Energy, Washington, DC.
Pub. in Jnl. of Chemical Education 63, n5 p452 1986.

Keywords: *Temperature measuring instruments, Miniaturization, Reprints.

A miniature mercury contact switch for use in undergraduate chemistry teaching laboratories is presented. Details of construction of the switch are provided, as well as the circuit used with the switch. The advantages of the switch are discussed, in addition to some suggested applications.

*600,974*
**PB87-107348** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Measurement Assurance Programs In a Field Environment.**
Final rept.,
W. G. Eicke, T. F. Leedy, B. R. Moore, and C. F. Brown. Mar 83, 5p
Sponsored by Army Missile Command, Redstone Arsenal, AL.
Pub. in National Conference of Standards Laboratories Newsletter 23, n1 p51-55 Mar 83.

Keywords: *Electrical measurement, Electric potential, Electric currents, Electrical resistance, Reprints.

To date most measurement assurance programs have been carried out between the National Bureau of Standards and various standards laboratories in the U.S. For the most part, these have been conducted at the highest accuracy levels. In the spring of 1982 the Army Missile Command and NBS conducted two special, lower accuracy, measurement assurance programs (S-MAP) at a field location at Redstone Arsenal, Alabama, in the areas of dc voltage, dc current, dc resistance, ac voltage, and ac current. The paper describes the experiments performed, presents the results, and discusses them in light of a number of externally imposed constraints.

*600,975*
**PB87-108106** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Time-Resolved Magnetic Dispersion for Large Isotope Ratio Measurements in Resonance Ionization Mass Spectrometry.**
Final rept.,
J. D. Fassett, H. J. Zeininger, and L. J. Moore. 1986, 12p
Pub. in International Jnl. of Mass Spectrometry and Ion Processes 69, p285-296 1986.

Keywords: *Spectrometers, *Measurement, Isotopes, Ionization, Abundance, Sensitivity, Ion beams, Dispersions, Ratios, Reprints, Laser applications.

The principle of time-resolved magnetic dispersion of ions can be used to improve the abundance sensitivity for elemental ratio measurement with laser ionization. A pulsed laser tuned to a discrete electronic transition of an element efficiently and selectively produces a pulsed ion beam. The pulsed ion beam is focused through a magnetic sector and, thus, mass filtering due to time-of-flight dispersion and magnetic dispersion is combined. The time-resolved magnetic dispersion is demonstrated using rhenium. The origin of scattered ions which cause loss of abundance sensitivity is displayed graphically in the magnetic field/time plane. Increased abundance sensitivity is demonstrated using tantalum.

*600,976*
**PB87-108155** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Development of a Temperature Compensated PVDF Transducer for Dynamic Pressure Measurements.**
Final rept.,
A. J. Bur, and S. C. Roth. 1984, 8p
Pub. in 1984 Annual Report--Conference on Electrical Insulation and Dielectric Phenomena, Wilmington, DE., October 21-25, 1984, p423-430.

Keywords: *Transducers, Dynamic pressure, Measurement, Temperature, Compensation, Thin films, Vinylidene chloride resins, Thermocouples, Adiabatic compression heating.

The pressure sensing element of the transducer is a thin film of polyvinylidene fluoride. The transducer is designed to measure dynamic pressures in the presence of thermal pulses which are produced by adiabatic compressional heating of the PVDF and its surroundings. Adiabatic heating of the PVDF will reduce its charge output by a constant 8%. Adiabatic heating of the surroundings will vary with each environment. Two approaches to compensating for environmental compressional heating are used.

*600,977*
**PB87-108569** PC **A14**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Specifications, Tolerances, and Other Technical Requirements for Weighing and Measuring Devices as Adopted by the 71st National Conference on Weights and Measures, 1986 (1987 Edition),**
O. K. Warnlof. Sep 86, 305p NBS/HB-44
Supersedes PB86-130358.Also available from Supt. of Docs as SN003-003-02755-3.

Keywords: *Weight indicators, *Measuring instruments, *Handbooks, Specifications, Tolerances(Mechanics), Requirements, Standards.

Handbook 44 was first published in 1949, having been preceded by similar handbooks of various designations and in several forms beginning in 1918. The 1987 edition was developed by the Committee on Specifications and Tolerances of the National Conference on Weights and Measures, with the assistance of the Office of Weights and Measures of the National Bureau of Standards. It includes amendments adopted by the 71st annual meeting of the National Conference on Weights and Measures in 1986. Handbook 44 is published in its entirety each year following the annual meeting of the National Conference on Weights and Measures.

*600,978*
**PB87-110094** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Machine Representation of Standards.**
Final rept.,
R. N. Wright, and J. W. Lyons. Aug 86, 5p
Pub. in ASTM Standardization News 14, n8 p44-48 Aug 86.

Keywords: *Standards, Reprints.

No abstract available.

*600,979*
**PB87-112298** PC **A06**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Semiconductor Measurement Technology: A Bibliography of NBS (National Bureau of Standards) Publications for the Years 1962-1985,**
J. Walters. Oct 86, 107p NBSIR-86/3464

Keywords: *Measurement, *Semiconductor devices, Bibliographies, Metrology, Gallium arsenides, Insulation, Interfaces, Integrated circuits, Packaging, National Bureau of Standards, Listings.

The bibliography contains reports of work performed at the National Bureau of Standards in the field of Semiconductor Measurement Technology in the period from 1962 through December 1985.

*600,980*
**PB87-113593** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Pulsed Laser Caliper for Noncontact Dimensional Measurement.**
Final rept.,
T. R. Lettieri. 1986, 7p
Pub. in Applied Optics 25, n9 p1443-1449, 1 May 86.

Keywords: *Dimensional measurement, Optical equipment, Reprints, *Laser applications, Noncontact measurement.

A new optical device for making caliperlike noncontact dimensional measurements on macroscopic objects is described. The device called a pulsed laser caliper, consists of a picosecond pulse laser, an ultrafast detector, various optical components, and a time-interval counter or high-speed sampling oscilloscope. Basically, a dimensional measurement is made by determining the time-of-flight difference between a reference laser pulse and another pulse which reflects off both sides of an object. Accuracy and limitations of the device are discussed briefly. Experimental results using a mode-locked argon laser and a sampling oscilloscope for pulse timing gave an accuracy of 0.075 cm in dimensional measurements of five gauge blocks with lengths from 1.9 to 10.2 cm.

*600,981*
**PB87-116091** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Force Callbration at the National Bureau of Standards.**
Final rept.,
R. A. Mitchell. Aug 86, 30p NBS/TN-1227
Also available from Supt. of Docs as SN003-003-02764-2.

Keywords: *Loads(Forces), *Calibrating, Measurement, National Bureau of Standards.

Force calibration and force measurement services available at the National Bureau of Standards (NBS) are described. Direct deadweight calibration of force sensors are performed in both compression and tension up to one million lbf (4.4 MN). Comparison calibrations relative to force sensor transfer standards are performed in compression up to 12 million lbf (53 MN). In addition to force calibrations, the following tests are performed to further characterize force sensors: temperature sensitivity, pressure sensitivity, creep, and eccentric load sensitivity.

*600,982*
**PB87-118154** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.

## Laboratory & Test Facilities

**High-Accuracy Automated Resistance Bridge for Measuring Quantum Hall Devices.**
Final rept.,
B. F. Field. 1985, 3p
Pub. in Institute of Electrical and Electronics Engineers Transactions on Instrumentation and Measurement IM-34, n2 p320-322 Jun 85.

Keywords: *Resistance bridges, *Hall effect, Measurement, Accuracy, Semiconductor devices, Comparison, Electrical resistance, Reprints.

An automated resistance bridge has been constructed specifically to measure the Hall resistance of semiconductor devices which exhibit the quantum Hall effect. The bridge is used to perform a one-to-one comparison of the Hall resistance to a reference resistor of similar value. A measurement accuracy of 0.01 ppm or better is expected.

*600,983*
**PB87-118162** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Sub-ppm Automated 1-10 Volt DC Measuring System.**
Final rept.,
B. F. Field. 1985, 4p
Pub. in Institute of Electrical and Electronics Engineers Transactions on Instrumentation and Measurement IM-34, n2 p327-330 1985.

Keywords: *Voltage measuring instruments, Calibrating, Accuracy, Voltmeters, Standards, Direct current, Reprints.

An automated measuring system has been developed for calibrating arbitrary-voltage references in the range one to ten volts with an inherent measurement accuracy of : or - 0.22 ppm (3 omega). The paper discusses the design and uncertainty analysis of the system and presents data obtained on an available Zener voltage reference.

*600,984*
**PB87-118774** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Calibration and Use of Optical Straight-Edges in the Metrology of Precision Machines.**
Final rept.,
W. T. Estler. 1985, 8p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Optical Engineering 24, n3 p372-379 1985.

Keywords: *Metrology, *Optical measuring instruments, Calibrating, Machine tools, Reprints.

The authors describe techniques used to measure straightness errors of precision machines. These measurements employ a dimensionally stable mechanical reference surface which is sampled with a laser interferometer - hence the term optical straightedge. The figure error of the reference surface and the straightness error motion of a coordinate measuring machine carriage in a horizontal plane are each measured with an estimated accuracy of 0.5 microinches (13 nm) over 40 inches (lm) of travel. When measuring straightness error in a vertical plane, the optical straightedge is deformed by gravitational forces. The authors use a computational algorithm, based upon simple beam theory, to correct straightness data for this distortion.

*600,985*
**PB87-118840** PC **A12**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Report of the National Conference on Weights and Measures (71st), 1986.**
Final rept.,
A. D. Tholen, C. S. Brickenkamp, and A. P. Heffernan. Sep 86, 273p NBS/SP-725
See also PB86-150232. Also available from Supt. of Docs as SN003-003-02765-1. Library of Congress catalog card no. 26-27766.

Keywords: *Meetings, *Metrology, *Weight measurement, Measurement, Evaluation, Education, Tests, Electromagnetic interference.

Reports by the several standing and annual committees of the Conference comprise the major portion of the publication. Included also are papers presented by Conference officials and others. Major issues discussed at the Conference included the National Type Evaluation Program, the National Training Program, compliance test methods for products subject to moisture loss, an electronic bulletin board, new methods of sale, electromagnetic interference on weights and measures devices.

*600,986*
**PB87-129003** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Note on the Results of the First Phase of an International Comparison in the Pressure Range 20 - 100 MPa Organized by the High-Pressure Working Group of the Comite Consultatif pour la Masse.**
Final rept.,
J. C. Legras, V. E. Bean, J. Jager, S. L. Lewis, and G. F. Molinar. 1985, 3p
Pub. in Jnl. of Physics E: Scientific Instruments 18, n4 p361-363 1985.

Keywords: *Pressure measurement, Comparison, Reprints, High pressure.

An international intercomparison in the pressure range 20 - 100 MPa has been organized under the auspices of the International Bureau of Weights and Measures. Given here is a brief outline of the results of the first of three phases in which the national standards laboratories of France, Italy, the United Kingdom, the United States of American and West Germany participated. These results show good agreement when considered in conjunction with the estimates of the uncertainty of measurement.

*600,987*
**PB87-134888** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**National Basis of Accuracy in Humidity Measurements.**
Final rept.,
S. Hasegawa. 1985, 14p
Pub. in Proceedings of International Symposium on Moisture Humidity, p15-28 1985.

Keywords: *Standards, *Humidity, Moisture meters, Accuracy, Hygrometers, Chemical analysis.

The paper summarizes the activities in humidity standards at the National Bureau of Standards (NBS). Included in the discussion will be brief descriptions of the standard hygrometer, saturation vapor pressure formulations, enhancement factors, humidity generators, secondary standard hygrometers and humidity fixed points using saturated salt solutions.

## Manufacturing Processes & Materials Handling

*600,988*
**PB86-193315** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Modeling the Optical Microscope Images of Thick Layers for the Purpose of Linewidth Measurement.**
Final rept.,
C. P. Kirk, and D. Nyyssonen. 1985, 9p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers 538, p179-187 1985.

Keywords: *Dimensional measurement, *Line width, Metal oxide transistors, Optical microscopes.

A monochromatic, waveguide model is presented which can predict the optical microscope images of thick-layer objects including multilayer structures with sloping, curved, and undercut edges, granular structures such as polysilicon, and asymmetric objects. The model is used to illustrate the effects of line structure on the optical image. Qualitative agreement with experimentally obtained optical image profiles is demonstrated. Application of the model to study the effects of variations in layer thickness and edge geometry on linewidth measurements made at different stages of manufacturing an MOS device is discussed.

*600,989*
**PB86-201399** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Electrodeposition of Nickel-Chromium Alloys.**
Final rept.,
D. S. Lashmore, and I. Weisshaus. 1984, 10p
Pub. in Proceedings of the Meeting of the Mechanical Failures Prevention Group (37th), Gaithersburg, MD., May 10-12, 1983, p39-48 1984.

Keywords: *Electrodeposition, Nickel alloys, Chromium alloys, Protective coatings, Wear resistance.

A process has been developed to electrodeposit nickel chromium alloys from aqueous solutions. The composition of this coating can be varied from 1% to about 60% (wt.) chromium by varying the deposition parameters. Coatings greater than 100 micrometers have been made. Dry sliding wear performance of the 20% chromium alloys is shown to be superior to electrodeposited nickel. The corrosion performance was characterized by the Potentiodynamic method. The alloy is a composition modulated materal with layers rich in chromium adjacent to layers poor in chromium. The layer spacings vary from between 100 and 1000 nanometers. The existence of layers is consistent with diffusion phenomena occurring in a two component system. These layers are thought to play a role in the corrosion performance of the coating.

## Nondestructive Testing

*600,990*
**PB86-158003** PC **A06**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**NVLAP (National Voluntary Laboratory Accreditation Program) Directory of Accredited Laboratories, 1985-86,**
H. W. Berger. Jan 86, 117p NBSIR-86/3315
See also PB85-178317.

Keywords: *Directories, *Laboratories, Test facilities, Accreditation.

The 1985-86 NVLAP Directory of Accredited Laboratories provides information on the activities of the National Bureau of Standards in administering the National Voluntary Laboratory Accreditation Program (NVLAP) during calendar year 1985. The status of current programs is briefly described and a summary of laboratory participation is provided. Indexes cross reference the laboratories by name, NVLAP Lab Code Number, test method, accreditation program, and geographical location and cross reference NVLAP code numbers with test method designations. The scope of accreditation of each laboratory, listing the test methods for which it is accredited, is provided along with a tabulation of test methods and the laboratories accredited for those test methods.

*600,991*
**PB86-160553** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Comparing EM (Electromagnetic) Susceptibility Measurement Results Between Reverberation and Anechoic Chambers.**
Final rept.,
M. L. Crawford, and G. H. Koepke. Aug 85, 9p
Sponsored by Naval Surface Weapons Center, Dahlgren, VA., and Rome Air Development Center, Griffiss AFB, NY.
Pub. in Proceedings of the IEEE (Institute of Electrical and Electronic Engineers) International Symposium on Electromagnetic Compatibility, Wakefield, MA., August 20-22, 1985, p152-160.

Keywords: *Anechoic chambers, Measurement, *Reverberation chambers, *Electromagnetic susceptibility.

The paper compares measurement results obtained using a 2.7 m x 3.1 m x 4.6 m reverberation chamber and a 4.9 m x 6.7 m x 8.5 m anechoic chamber to determine the EM susceptibility of equipment under test (EUT). The frequency range was 200 MHz - 18 GHz. The 'correlation factor' between the two techniques appears to be directly proportional to the gain of the EUT. Four sample EUTs included in the study were a one centimeter dipole probe, a ridged horn antenna, a small rectangular TEM transmission cell with an aperture and a modified 7.0 cm (2.75n) diameter folded fin aircraft rocket.

*600,992*
**PB86-163474** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Weld Flaw Sizing Using Back-Scattered and Forward-Scattered Low Frequency Ultrasound.**
Final rept.,
R. E. Schramm, and T. A. Siewert. Nov 85, 8p
Sponsored by Ames Lab., IA.
Pub. in Proceedings of World Conference on Nondestructive Testing (11th), Las Vegas, NV., November 3-8, 1985, p1286-1293.

Keywords: *Ultrasonic tests, *Weld defects, Transducers.

Electromagnetic-acoustic transducers (EMATs) generating low frequency ultrasound can detect and size planar flaws in welds. The back-scattered signal carries information on the through-depth flaw size. Measurements on slits in 16-mm thick steel plates indicated a sensitivity to flaw depth sizes as small as 0.5 mm. In accordance with theory, the signal saturated at about 2.5 mm. This is a very important size range for many fracture mechanics considerations, but it is desirable to extend the range to still larger flaw sizes. The report describes the simultaneous use of the forward and back-scattered signals to extend the range. Processing the signals from two receiver transducers on either side of the flaw demonstrated a sizing ability for artificial flaws up to 11-mm deep. The technique has also been successfully applied to two welded plates, each containing intentional flaws such as inadequate joint penetration and incomplete fusion. The weld flaw sizes predicted by the EMAT signals and those determined by destructive metallography agree within 1 mm.

*600,993*
**PB86-181369** PC **A99**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Thermometry.**
Final rept.,
J. F. Schooley. Mar 86, 634p NBSIR-85/3133

Keywords: *Temperature measurement, *Thermometry, *Thermometors.

The manuscript develops the concept of thermometry, including historical experiments and thermodynamics; the Kelvin thermodynamic temperature scale; international practical temperature scales; the thermodynamic methods used to realize the Kelvin scale; and modern types of thermometers. Nearly 400 bibliographic references are included.

*600,994*
**PB86-182375** PC **A10**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.
**Institute for Materials Science and Engineering, Nondestructive Evaluation: Technical Activities 1985.**
Annual rept.,
H. T. Yolken, L. Mordfin, and G. Birnbaum. Nov 85, 220p NBSIR-85/3187
See also PB84-217074.

Keywords: *Nondestructive tests, *Standards, Composite materials, Process control, Interfaces.

A review of the Nondestructive Evaluation Program at NBS, for fiscal year 1985, is presented in the annual report.

*600,995*
**PB86-200953** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**International Organization of Legal Metrology.**
Final rept.,
D. R. Mackay. 1983, 5p
Pub. in Proceedings of Annual Conference Standards Engineering Society: The Spectrum of Evolving Standards, Dayton, OH., September 26-28, 1983, p44-48.

Keywords: *Metrology, *Organizations, Recommendations, Standards, International relations, *Legal metrology.

The International Organization of Legal Metrology (OIML) was founded in 1955 to promote intergovernmental cooperation in the field of legal metrology. The United States joined this organization in 1972 and the National Bureau of Standards was assigned the responsibility for managing the U.S. involvement in cooperation with the Department of State. The paper describes the functions of the International Conference of Legal Metrology, the International Committee of Legal Metrology, and the International Bureau of Legal Metrology. The organizational procedures for the development and approval of International Recommendations through the Pilot Secretariats and the Reporting Secretariats. The U.S. involvement and participation in the technical programs of OIML is discussed as well as the importance of both public and private sector participation in terms of the future exportation of U.S. manufactured products.

*600,996*
**PB86-202082** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Status of NBS (National Bureau of Standards) Recognition of Calibration Capabilities.**
Final rept.,
J. W. Locke. 1983, 6p
Pub. in Proceedings of the National Conference of Standards Laboratories Workshop and Symposium (1983), Boulder, CO., July 18-21, 1983, p2.6A.1--2.6A.6.

Keywords: *Calibrating, National Bureau of Standards.

Describe the status of efforts at NBS related to domestic and international recognition of U.S. calibration facilities.

*600,997*
**PB86-238359** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Mossbauer Techniques in Nondestructive Evaluation.**
Final rept.,
L. H. Bennett. 1986, 4p
Pub. in Encyclopedia of Materials Science and Engineering, v4 p3121-3124 1986.

Keywords: *Nondestructive tests, *Mossbauer effect, Materials tests, Reprints.

The Mossbauer effect, a nuclear-physics technique involving the emission and resonant absorption of gamma rays without recoil, is also known as nuclear gamma-ray resonance or nuclear resonance-fluorescence. It provides information on the local atomic environment which, in turn, relates to the properties of the materials. Mossbauer studies have been applied to a wide variety of problems, including catalysis, corrosion, magnetism, atomic structure, chemical kinetics, diffusion and biology. Many nuclear isotopes can be used for Mossbauer studies, but the most common is 57 Fe. For the reason, nondestructive evaluation studies in ferrous metallurgy is an important applications area for the Mossbauer technique.

*600,998*
**PB86-238383** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Failure Analysis: Nondestructive Evaluation.**
Final rept.,
B. W. Christ. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v3 p1617-1619 1986.

Keywords: *Nondestructive tests, Failure, Pressure vessels, Ultrasonic tests, Radiography, Inspection, Reprints.

The role of NDE in failure analysis is discussed. Some applications of the State-of-the-Art are described.

*600,999*
**PB86-239381** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Microwave Nondestructive Evaluation.**
Final rept.,
D. A. Ellerbruch. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v4 p3050-3054 1986.

Keywords: *Nondestructive tests, Electromagnetic tests, Microwaves, Scattering, Reprints.

The electromagnetic equations relevant to microwave nondestructive evaluation are given in this review paper. Microwave signal scattering and measurements in the time and frequency domain are discussed with respect to real measurement situations.

*601,000*
**PB86-240785** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Texture: Nondestructive Characterization.**
Final rept.,
H. J. Prask, and C. S. Choi. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v7 p4895-4897 1986.

Keywords: *Texture, *Nondestructive tests, *Materials tests, Anisotropy, Orientation, Diffraction, Reprints.

Texture is the term applied to the presence of a preferred crystallographic orientation of the crystallites (grains) in a polycrystalline material. Fibers become textured during growth or processing. Mechanical operations such as drawing, rolling or swaging induce texture. All such texturing introduces anisotropy in the mechanical properties of the aggregate which affects the response of the material during further forming, fabrication or in-service operations.

*601,001*
**PB86-241759** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of Nondestructive Evaluation.
**Residual Stresses: Nondestructive Evaluation.**
Final rept.,
L. Mordfin. 1986, 7p
Pub. in Encyclopedia of Materials Science and Engineering, v6 p4188-4194 1986.

Keywords: *Nondestructive tests, *Materials tests, Residual stress, X ray diffraction, Ultrasonic tests, Barkhausen effect, Neutron diffraction, Determination of stress, Reprints.

Following a brief description of the nature and the significance of residual stresses in materials, the physical bases of nondestructive methods for measuring residual stresses are presented. Principal emphases are on the conventional x-ray diffraction method and on the ultrasonic method. An approach based on Barkhausen noise analysis is briefly described. Recent research on the measurement of internal stresses by neutron diffraction and by high-energy x-ray diffraction is noted.

*601,002*
**PB86-241965** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Optical Nondestructive Evaluation.**
Final rept.,
E. C. Teague, T. V. Vorburger, and G. Birnbaum. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v5 p3312-3316 1986.

Keywords: *Nondestructive tests, *Optical tests, Surface properties, Reprints.

The review deals with optical techniques for evaluating the surface flaws and surface roughness of solids, in short, the quality of solid surfaces. The wide variety of optical NDE techniques have been grouped into four classes; imaging, scattering, diffraction, and profiling. An illustrative example of each class is discussed and opto-acoustic NDE methods are briefly reviewed.

*601,003*
**PB86-242575** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Magnetic Nondestructive Evaluation.**
Final rept.,
L. J. Swartzendruber. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v4 p2694-2698 1986.

Keywords: *Nondestructive tests, *Magnetic tests, Magnetic fields, Magnetic properties, Reprints.

Magnetic methods of nondestructive evaluation utilize the relationship between material properties and static or slowly varying magnetic fields. They find wide application both on the production line and in the field and, where useable, provide a sensitive, rapid, and often relatively inexpensive test method. Uses include measurement of important metallurgical properties, detection of harmful defects, and measurement of coating thickness. This article will briefly review the properties of leakage fields and methods of their de-

tection and the origin and measurement of magnetic properties.

*601,004*
**PB87-104428** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Investigation of the Use of Nondestructive Methods for Inspection of Seams of Single-Ply Roofing Membranes,**
W. J. Rossiter. Sep 86, 36p NBSIR-86/3455
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Roofing, Detection, Ultrasonic tests, Seams(Joints), Nondestructive tests, Inspection, *Infrared thermography.

Investigations were conducted regarding the use of the ultrasonic pulse echo and the infrared thermography nondestructive evaluation (NDE) methods for detecting voids and delaminations in adhesive-bonded seams of single-ply roofing membranes. Results indicated that the ultrasonic pulse echo method using a wheel transducer can be useful as a field technique for assisting in the quality assessment of seams.

*601,005*
**PB87-115432** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Mapping of Eddy Current Probe Fields.**
Final rept.,
T. E. Capobianco, F. R. Fickett, and J. C. Moulder. 1986, 7p
Pub. in Review of Progress in Quantitative Nondestructive Evaluation 5A, p705-711 1986.

Keywords: *Eddy current tests, Magnetic fields, Electrical measurement, Nondestructive tests, Mapping, Probes, Eddy currents.

The magnetic fields produced by four different eddy current probes were mapped in the near field with very small (0.43) mm dia inductive magnetic field sensors. The four eddy current probes included two nominally identical, absolute, air core probes, an absolute ferrite core probe, a reflection probe with an air core excitation coil and two counterwound ferrite core pickup coils. Measured fields for the air core probes are compared with values calculated from the theory of Dodd and Deeds. All measurements were performed at 10 kHz; for the ferrite core probe the field intensity was also measured from 1 kHz to 100 kHz using conventional methods.

*601,006*
**PB87-118766** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Inverse Problem of Acoustic Emission - Explicit Determination of Acoustic Emission Source Time-Functions.**
Final rept.,
N. N. Hsu, and D. G. Eitzen. 1982, 8p
Pub. in Review of Progress in Quantitative Nondestruction Evaluation 1, p405-412 1982.

Keywords: Signal processing, Reprints, *Acoustic emission testing.

The paper addresses the problem of determining the AE source time-function from the detected AE signal with a sensor located a short distance away from the source. The solution to the problem is in the form of an inverse filter (deconvolution filter) such that the explicit waveform of the source can be obtained by passing the detected AE signal through such a filter. In other words, by removing the effects of the reverberations of the structure and the particular characteristics of the sensor, the filter recovers the AE source signature which characterizes the source mechanism alone.

*601,007*
**PB87-122206** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Acoustic Emission Chip-Form Monitor for Single-Point Turning.**
Final rept.,
K. W. Yee, D. S. Blomquist, D. A. Dornfeld, and C. S. Pan. 1986, 8p
Pub. in Proceedings of International Machine Tool Design and Research Conference (26th), Manchester, England, September 17-18, 1986, p305-312.

Keywords: Microcomputers, Algorithms, Chips, Breaking, Aluminum, Steels, Alloy steels, Machine tools, *Acoustics emissions, *Chips(Electronics), *Computer aided manufacturing, Monitoring.

An acoustic-emission-based microcomputer chip-form monitor has been designed and built at the National Bureau of Standards (NBS). The monitor implements algorithms based on research by the University of California, Berkeley. The ability to identify chip form in turning of three types of metal (aluminum, low-carbon steel, and an alloy steel) has been demonstrated at both institutions, each using different machine tools and different tooling. The monitor performs best for the soft, east-to-machine metals where chip breaking is most difficult and disastrous tangles are most likely.

*601,008*
**PB87-131470** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Flaw Detection with a Magnetic Field Gradiometer.**
Final rept.,
T. E. Capobianco, J. C. Moulder, and F. R. Fickett. 1985, 6p
Pub. in Proceedings of Symposium on Nondestructive Evaluation (15th), San Antonio, TX., April 23-25, 1985, p15-20.

Keywords: *Eddy current tests, Nondestructive tests, Magnetic measurement, SQUID devices, Gradiometers, Defects(Materials).

When eddy currents are induced in a conductor, flaws deflect the eddy currents and perturb the associated electric and magnetic fields. In conventional eddy current testing, the perturbed fields associated with a flaw are detected as a change in the impedance of the test coil used to induce the eddy currents. More direct methods for detecting and characterizing flaw-perturbed fields, both electric and magnetic, have also been developed. The authors describe a method for determining the normal component of the magnetic field gradient caused by a flaw. A novel feature of the measurement system is the use of a Superconducting Quantum Interference Device (SQUID). The SQUID provides more sensitivity than conventional detection methods, and the possibility of calibration based on a fundamental physical quantity: the flux quantum. Results are reported of a series of measurements on a fatigue crack and several manufactured defects in aluminum alloy specimens using the system. The effect of edge proximity compared to flaw signal and a figure of merit are also discussed.

*601,009*
**PB87-132049** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Rayleigh Wave Propagation in Deformed Orthotropic Materials.**
Final rept.,
P. P. Delsanto, and A. V. Clark. 1986, 9p
Pub. in Review of Progress in Quantitative Nondestructive Evaluation 5B, p1407-1414 1986.

Keywords: *Orthotropic plates, Surfaces, Propagation, Anisotropy, Nondestructive tests, Reprints, *Rayleigh waves.

A perturbation method is described for the investigation of the propagation of Rayleigh waves on the surface of a homogeneous anisotropic initally deformed material plate. The authors derive the Rayleigh wave phase velocity as a function of the propagation direction, the elastic constants and the initial stresses. The linearity of our formulas suggests that Rayleigh waves can be conveniently used as an experimental technique for the solution of the inverse problem of determining the elastic constants and/or the initial stresses in the material. The perturbation formalism is quite general and can be applied whenever other small effects, like slight temperature changes or external magnetic fields, affect the Rayleigh wave propagation velocity.

*601,010*
**PB87-136701** PC **A05**/MF **A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Institute for Materials Science and Engineering, Fracture and Deformation: Technical Activities 1986.**
Oct 86, 77p NBSIR-86/3436
See also PB86-182375.

Keywords: *Deformation, *Nondestructive tests, *Fractures(materials), Fracture tests, Stress analysis, Fracture properties, Crack propagation, Welding, Cracking(Fatigue), Metallurgy, Composite materials, Grain boundaries, Mechanical properties, Technical activities.

The report summarizes the technical program of the Fracture and Deformation Division of the Institute for materials Science and Engineering, National Bureau of Standards for the fiscal year 1986. The division's two major program areas are elastic-plastic fracture mechanics and fracture mechanisms and analysis. Elastic-plastic fracture mechanics includes contributions from stress analysis, material properties, nondestructive evaluation, and welding. Division efforts in fracture physics, time-dependent properties, composite mechanics, mechanical metallurgy, physical properties, and material performance compose the second area, fracture mechanisms and analysis. Significant technical programs relating to each of these are presented. Major accomplishments are highlighted, including an interdisciplinary analysis of a major pressure vessel failure, extensive collaboration with the automotive industry to reduce costs associated with failure, successful large-scale experiments of dynamic crack arrest, and composite-modeling, material-property, and test-development research.

## Production Planning & Process Controls

*601,011*
**AD-P003 180/7** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Washington, DC. Center for Mfg. Engineering.
**Data Distribution in the NBS (National Bureau of Standards) Automated Manufacturing Research Facility,**
M. J. Mitchell, and E. J. Barkmeyer. 1984, 17p
Pub. in Proceedings IPAD II, Advances in Distributed Data Base Management for CAD/CAM, National Symposium Held in Denver, CO. on 17-19 Apr 84, AD-A140 614, p211-227.

Keywords: *Manufacturing, *Automation, *Research facilities, Data management, Data bases, Distributed data processing, Systems analysis, Computer architecture, Interfaces, Networks, Research management, Technology transfer, Computer aided design, Component Reports, NBS(National Bureau of Standards), Distributed data dictionaries, CAM(Computer Aided Manufacturing).

The NBS(National Bureau of Standards) AMRF(Automated Manufacturing Research Facility) exemplifies one approach to integrating a set of heterogeneous distributed databases. While the 1983 implementation is primitive, it provides real-time control processes with access to conventional databases, rapidly changing memory-resident data, and large binary files. It demonstrates the feasibility of front-ending existing data management systems with a Data Administration System implementing a common user interface, constructing process-dependent logical views of the data, and providing networked data access. The major shortcoming of the current implementation is the absence of a common data dictionary, and the major task of the near future is the development and automation of a distributed data dictionary system.

*601,012*
**PB86-201738** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Acoustic Emission for In-Process Monitoring and Microstructure Control.**
Final rept.,
H. N. G. Wadley, and R. Mehrabian. 1984, 10p
Pub. in Proceedings of the Determ. Nondestr. Methods Mater., p26-27 1984.

Keywords: *Process control, *Metal finishing, Quality control, Microstructure, Cracking(Fracturing), Phase transformations, Plastic properties, Acoustic emissions, *Acoustic emission testing.

Acoustic emissions are the elastic waves emitted by sudden localized changes of stress by, for example, the formation of cracks, plasticity, and phase transfor-

mations. It is beginning to be considered a potential in-process monitoring technique for quality and productivity improvement as a sensor for closed loop feedback control systems. Applications of the technique are held back because of its complicated nature and because the signals are controlled rather subtly by microstructure. In the review the authors describe the theoretical framework that has begun to emerge and which now provides a physical understanding of acoustic emission. The authors then reconsider the results of laboratory studies and recent applications to assess, in the light of this understanding, the contribution acoustic emission methods might make toward in-process monitoring and microstructure control during metals processing.

## Quality Control & Reliability

*601,013*

**PB86-202025** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**What Is Quality Assurance.**
Final rept.,
J. K. Taylor. 1985, 7p
Pub. in Proceedings of the Quality Assurance for Environmental Measurements Symposium, Boulder, CO., August 8-12, 1983, ASTM (American Society for Testing and Materials) Spec. Tech. Pub. 867, p5-11 1985.

Keywords: *Quality assurance, *Data processing, Accuracy, Quality control, Data.

The quality of data must be known and established before it can be used logically in any application. Data quality may be judged on the basis of its quantitative accuracy and on the confidence that can be placed in the qualitative identification of the parameters measured. This requires its production in a quality assurance program that permits the assignment of its statistically supported limits of uncertainty. The essential features of such a program, consisting of quality control and quality assessment techniques, are discussed in the paper.

## Tooling, Machinery, & Tools

*601,014*

**PB87-118741** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Centrifugal Pump for Superfluid Helium.**
Final rept.,
W. G. Steward. 1986, 6p
Pub. in Cryogenics 26, p97-102 Feb 86.

Keywords: *Centrifugal pumps, Cryogenics, Liquid helium, Superfluidity, Reprints.

The paper summarizes and correlates the liquid helium pump data obtained previously in two separate test programs. In normal helium the second set of data shows a large performance improvement over the first set as a result of changes in measurement methods and in the pump itself. Peak pump efficiencies of 46% were measured. The pump appeared to perform approximately the same in He II as in He I; however, the He II data are not adequate for system design or analyses. Therefore, a new pump test program is planned to test the improved version of the pump in an apparatus designed specifically for He II.

## General

*601,015*

**N86-29155/6** PC A05/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Stability of Some Epoxy-Encapsulated Diode Thermometers.**
B. W. Mangum, and G. A. Evans. Feb 86, 99p NAS 1.26:178137, NBSIR-86-3337, NASA-CR-178137 NASA ORDER-L-83949B

Keywords: *Diodes, *Epoxy compounds, *Temperature effects, *Temperature gradients, *Thermometers, Airfoils, Calibrating, Cryogenics, Surface temperature, Temperature measurement.

The stability upon thermal cycling and handling of ten small, epoxy-encapsulated silicon diode thermometers at six temperatures in the range from liquid nitrogen temperatures to about 60 C. The nominal temperatures of measurement were -196, -78, 0, 20, 40, and 60 C, as measured on the International Practical Temperature Scale of 1968. Diodes were to be thermally cycled 15 to 20 times. Since NASA anticipates that the uncertainty in their temperature measurements will be + or - 50 mK, uncertainties as large as + or - 10 mK in the measurements of the evaluaton can be accommodated without deleteriously affecting the value of the results of the investigation.

*601,016*

**PATENT-4 576 486** Not available NTIS
Department of Commerce, Washington, DC.
**Optical Fiber Thermometer.**
Patent,
R. R. Dils. Filed 23 Aug 83, patented 18 Mar 86, 10p PB86-176575, PAT-APPL-6-525 771
Supersedes PB84-113760.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Temperature measuring instruments, *Patent application, Fiber optics, Ceramic fibers, Blackbody radiation, Photo dectors, PAT-CL-374-131.

A temperature measuring device suitable for high temperature measurements in the range of 500 - 2400 C. utilizing a blackbody cavity to emit radiation in the wavelength band of 0.3 microgram - 1.0 mircogram. The emitted light is transmitted to a photodector via a high temperature ceramic fiber which is transparent to the wavelength band radiated. The radiance of the cavity is utilized as a measure of its temperature.

*601,017*

**PATENT-4 577 510** Not available NTIS
Department of the Air Force, Washington, DC.
**Dynamic Polymer Pressure Transducer with Temperature Compensation.**
Patent,
A. J. Bur, and S. C. Roth. Filed 6 Sep 84, patented 25 Mar 86, 6p AD-D012 285/3, PAT-APPL-6-647 782
Supersedes PAT-APPL-6-647 782, AD-D011 373.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Patents, *Pressure transducers, *Pressure gages, Polyvinylidenes, Fluoropolymers, Dynamic pressure, Temperature, Compensation, Thermal properties, Thermocouples, Signals, Amplifiers, Circuits, Accuracy, Polyvinylidene fluoride, PAT-CL-73-708.

Accurate dynamic pressure data in a changing thermal environment is obtained through the use of a pressure gage formed from polyvinylidene fluoride (PVDF) polymer material. The temperature compensation pressure gage has three major elements: an active PVDF transducer which obtains remote pressure readings which are uncorrected for thermal effects; a thermocouple having a short rise time allowing an output thermal signal which dynamically responds to changing thermal conditions; and a compensation amplifier circuit receiving uncorrected pressure readings and the dynamic thermal signal and producing on output signal representing accurate pressure data which is corrected for changing thermal conditions. Also disclosed are the details of making an active PVDF transducer.

*601,018*

**PB86-160579** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Characterization of Polyvinylidene Fluoride Pressure Transducers.**
Final rept.,
A. J. Bur, and S. C. Roth. 1985, 6p
Pub. in Proceedings of the International Symposium on Electrets (5th), Heidelberg, West Germany, 1985, p712-717.

Keywords: *Pressure gages, Shear stress, Piezoelectricity, Meeting, *Vinylidene fluoride polymers.

The construction, calibration and use of a polyvinylidene fluoride (PVDF) pressure gage is described. The transducer material, PVDF, is in the form of 12 micrometer films with active areas 1 cm in diameter. The gage consists of two films whose active regions are laminated together face-to-face and subsequently laminated between protective layers of polycarbonate or another suitable polymer material. Temperature compensation, which is achieved by both active and passive techniques, is described. The response of the PVDF gage to shear stresses is found to be significant but small compared to the response to an equivalent hydrostatic pressure.

*601,019*

**PB86-162039** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Handling Blunt Flaws in a Fitness-for-Service Assessment of Pipeline Weld Quality.**
Final rept.,
M. B. Kasen, and G. E. Hicho. 1985, 16p
Pub. in Proceedings of the Fracture Mechanics Seminar School (3rd): Fracture Mechanics of Weldments, Apandelova, Yugoslavia, June 25-29, 1984, p339-354.

Keywords: *Welded joints, *Pipelines, *Weldments, Weld defects, Crack propagation, Fracture(Mechanics).

The significance of porosity, slag and arc burns on pipeline integrity is evaluated by assessing the probability of their contributing to crack initiation and to accelerated crack growth during low cycle fatigue. It is found that such flaws are essentially innocuous in tough weldments where failure is dominated by the geometric discontinuity created by the weld reinforcement. It is shown that the maximum through-wall depth of slag and porosity is limited to the depth of the weld pass in which they occur. This provides an upper limit to flaw depth that greatly simplifies assessment of flaw significance by fracture mechanics principles, should it be desired to do so. Suggestions are offered for approaches to treating the presence of blunt flaws during field inspections of pipelines.

*601,020*

**PB86-164555** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**Economic Model for Automatic Test Equipment Calibration.**
Final rept.,
S. F. Weber. 1985, 6p
Pub. in Proceedings of Autotestcon '85 IEEE (Institute of Electrical and Electronics Engineers) International Automatic Testing Conference, Long Island, NY., October 22-24, 1985, p347-352.

Keywords: *Calibrating, *Automatic test equipment.

A model for estimating the benefits of improved ATE calibration is presented and illustrated. The benefits are stated in terms of reduced probabilities of the two types of errors possible in every test situation: Consumer's Loss (CL) and Producer's Loss (PL). CL is the probability of accepting a bad unit under test (UUT) and PL is the probability of rejecting a good UUT. The model expresses both probabilities, CL and PL, as explicit functions of measurement bias (systematic error), represented by the mean of measurement error, and of measurement imprecision, represented by the standard deviation of measurement error. The model can directly translate any changes in bias and/or precision resulting from a calibration improvement into changes inthe probabilities, CL and PL. When applied to a case study, the economic value of the improvement, in terms of dollars saved per UUT tested, can be established from these probabilities.

*601,021*

**PB86-171139** PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

**Procedure for Calibration of Ferrite Gaps in Magnetic Tape Heads Traceable to NBS (National Bureau of Standards) AR-Chromium Optical Linewidth SRMs,**
D. Nyyssonen. Feb 86, 8p NBSIR-86-3306

Keywords: Dimensional measurement, Magnetic tapes, Calibrating, Line width.

Accurate calibration of micrometer and submicrometer optical line-width measuring systems requires that the calibration standard match the properties of the line to be measured. The NBS photomask linewidth standards have been designed for use by the integrated circuit community and are not directly suitable for use in other applications. A method of calibrating systems for measuring the width of ferrite gaps in magnetic tape heads has been developed that involves a two-step calibration using the NBS antireflecting-chromium photomask as the primary reference standard. This primary standard is used in transmitted green light to calibrate the linewidths on a secondary black-chromium photomask.

*601,022*
**PB86-177714** PC **A05**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Thermometer Calibration: A Model for State Calibration Laboratories.**
Final rept.,
J. A. Wise, and R. J. Soulen. Jan 86, 91p NBS/MONO-174
Also available from Supt. of Docs as SN003-003-02707-3. Library of Congress catalog card no. 85-600636.

Keywords: *Thermometers, Calibrating.

The document describes the means by which a state calibration laboratory can establish a calibration service based on liquid-in-glass thermometers. Discussed are: ice-point baths, controlled-temperature baths, thermometer inspection, calibration techniques, and control chart procedures.

*601,023*
**PB86-188497** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Heat-Pump Cycles with Refrigerant Non-Azeotropic Mixtures in Thermodynamic Diagrams.**
Final rept.,
R. Radermacher. 1984, 1p
Sponsored by Electric Power Research Inst., Palo Alto, CA.
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air Conditioning Engineers) Jnl. EN-26, n5 p52 1984.

Keywords: *Heat pumps, Distillation, Refrigerants, Thermodynamics, Reprints, Thermodynamic diagrams.

Various thermodynamic diagrams that are well known in absorption heat pump design and distillation techniques are introduced in the paper for non-azeotropic halogenated hydrocarbon mixtures. As an example, a typical compressor heat pump cycle for refrigerant mixtures is displayed and the cycle itself discussed using these diagrams. It is shown that virtually all the necessary thermodynamic design information can be obtained from the enthalpy-composition diagram. It offers the possibility to determine the amount of heat, pressures, temperatures and compositions involved by simple geometric constructions even when the refrigerant flow rate varies in certain components. Furthermore, it is shown by an example that thermodynamic diagrams provide a basic understanding of the influence of refrigerant properties on the heat pump cycle.

*601,024*
**PB86-192002** PC **A09**/MF **A01**
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Industrial Time Service Study,**
D. W. Hanson, and D. A. Howe. Feb 86, 194p NBSIR-86/3042
Sponsored by Bonneville Power Administration, Portland, OR.

Keywords: *Time standards, *Frequency standards, Accuracy, Time signals, Time dissemination, Time broadcast service.

The study examines options for delivery of accurate time and frequency information to industrial users. The study is sponsored by the Bonneville Power Administration (BPA) who finds a need for accurate timing to the one microsecond level. Prospective existing and future dissemination methods (Loran-C, GOES, USRDSS, GPS, etc.) are discussed in detail. The study produces a system architecture and preliminary design for a new time service using the widely available U.S. fixed satellite service (FSS) in which customers shall assume full costs of its operation through subscriber fees. The study elaborates on three viable options: (1) FSS, (2) GPS, and (3) USRDSS. Based on the study, conclusions can be drawn regarding a timing system which will most satisfactorily meet the long range goals of most industrial users.

*601,025*
**PB86-192127** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Toward an Efficient Operation of a Series Solar Heat Pump System.**
Final rept.,
T. Y. Bong. 1983, 11p
Sponsored by Department of Energy, Washington, DC.
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 89, pt2A-2B p617-627 1983.

Keywords: *Heat pumps, Solar energy, Efficiency, Temperature control, Reprints.

In operating a series solar heat pump system, a common practice is to use direct solar heating instead of the heat pump whenever the temperature of the solar-heated water exceeds a certain value called the switch-over temperature. The switch over temperature setting has a significant effect on the system's energy consumption. It is shown in the analytical study that the ideal switch-over temperature increases with the building load, but that it has a maximum value determined completely by the characteristics of the water-to-air heat pump. If because of its controller, a series solar heat pump system is to have a fixed switch-over temperature independent of the building load, then the temperature should not exceed the ideal switch-over temperature corresponding to the building design load if the energy consumption of the system is to be minimized.

*601,026*
**PB86-192234** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Brief History of Measurement Systems with a Chart of the Modernized Metric System.**
Final rept.,
D. Goldman. Mar 86, 6p NBS/SP-304A
See also PB86-192242. Also available from Supt. of Docs as SN003-003-02696-4.Color illustrations reproduced in black and white.

Keywords: *Metric system, *Units of measurement, Charts.

The chart presents a popularized yet technically accurate guide to SI base units, supplementary units, multiples and prefixes, and common conversions. The intended audience is (mainly) school children and the general public.

*601,027*
**PB86-192242** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Modernized Metric System (Chart).**
Final rept.,
D. Goldman. Mar 86, 22p NBS/SP-304
See also PB86-192234. Also available from Supt. of Docs as SN003-003-02695-6.Color illustrations reproduced in black and white.

Keywords: *Metric system, *Units of measurement, Charts.

The chart presents a popularized yet technically accurate guide to SI base units, supplementary units, multiples and prefixes, and common conversions. The intended audience is (mainly) school children and the general public.

*601,028*
**PB86-193109** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**International Laboratory Accreditation Conference.**
Final rept.,
S. I. Warshaw. Jan 86, 3p
Sponsored by American Society for Testing and Materials, Philadelphia, PA.
Pub. in ASTM (American Society for Testing and Materials) Standardization News 14, n1 p42-44 Jan 86.

Keywords: *Laboratories, Test facilities, Standards, Measurement, Meetings, Reprints, *Accreditation.

A description is given of the organization and activity of the International Laboratory Accreditation Conference. Included is a listing of respresentation from the United States, international organizations, and other nations.

*601,029*
**PB86-193604** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Measurement of the Silver Freezing Point with an Optical Fiber Thermometer: Proof of Concept.**
Final rept.,
R. R. Dils, J. Geist, and M. L. Reilly. 15 Feb 86, 8p
Pub. in Jnl. of Applied Physics 59, n4 p1005-1012, 15 Feb 86.

Keywords: *Melting points, *Silver, *Temperature measuring instruments, Gold, Reprints, *Thermometers, Optical fibers.

Measurements were made at the gold and silver freezing points to demonstrate the accuracy of the new optical fiber thermometer (OFT). It is shown that the output signal from the OFT is related to the radiance from a blackbody source in a simple manner, and that the temperature interval between the gold and silver freezing points, as determined with the OFT, is close to other recent results.

*601,030*
**PB86-195971** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Low-Cost Tubular Sapphire Optical-Cells for Study of Phase-Separation in Fluid Mixtures.**
Final rept.,
H. A. Davis. 1983, 2p
Pub. in Review of Scientific Instruments 54, n10 p1412-1413 1983.

Keywords: Laboratory equipment, Reprints, *Optical cells.

The construction of low-cost optical cells using the thin-walled sapphire tubing, which are used for observation of phase separation in fluid mixtures, are described.

*601,031*
**PB86-196763** PC **A05**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD.
**Measurement Evaluation.**
Special pub.,
J. Mandel, and L. F. Nanni. Mar 86, 77p NBS/SP-700/2
See also HRP-0029178. Also available from Supt. of Docs as SN003-003-02720-1. Library of Congress catalog card no. 86-600510.

Keywords: *Measurement, Evaluation, Statistical analysis, Quality control.

The paper was published originally as a chapter in the book entitled 'Quality Assurance Practices for Health Laboratories'. It is for that reason that the examples used as illustrations are taken from health-related fields of research. However, the statistical concepts and methods presented here are entirely general and therefore also applicable to measurements originating in physics, chemistry, engineering, and other technical disciplines. The reader should have no difficulty in applying the material of this paper to the systems of measurement in his particular field of activity.

*601,032*
**PB86-197365** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

**Temperature Distribution in the Diamond Anvil Pressure Cell at High Temperature.**
Final rept.,
R. G. Munro, S. Block, G. J. Piermarini, and F. A. Mauer. 1 Jan 84, 5p
Pub. in Jnl. of Applied Physics 55, n1 p4-8, 1 Jan 84.

Keywords: *Load cells, Diamonds, Temperature distribution, Thermal diffusion, Heating equipment, Reprints, Finite difference methods.

The temperature distribution in a diamond anvil pressure cell is investigated theoretically for a realistic model cell having a cylindrical external heater. For a heater surface at 1000 absolute degrees above the ambient temperature, it is found, at steady state, that the region of the sample chamber is, for all practical purposes, isothermal at a temperature of about 11 degrees below the temperature of the heater. When the heater temperature is subsequently incremented instantaneously by ten degrees, a new steady state is reached in about 30 seconds.

*601,033*
**PB86-201274** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**NBS (National Bureau of Standards) 50 kHz Phase Angle Calibration Standard.**
Final rept.,
R. S. Turgel. Apr 86, 85p NBS/TN-1220
Also available from Supt. of Docs as SN003-003-02726-0. Sponsored by Department of Defense Calibration Coordination Group, Redstone Arsenal, AL.

Keywords: *Phase angle, *Calibrating, Standards, Phase meters, Waveforms, Waveform generators.

A detailed description is given of the features of an electrical phase angle calibration standard designed for operation over a frequency span of 2 Hz to 50 kHz. The phase resolution of the calibrator extends from just below 2 millidegrees at the low end of the frequency range to about 5 millidegrees at the high end. The uncertainty in the phase angle is a function of frequency, amplitude, and amplitude ratio of the two outputs. It varies from 5-50 millidegrees.

*601,034*
**PB86-202108** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Iodine Stabilized Laser as a Realization of the Length Unit.**
Final rept.,
H. P. Layer. 1978, 1p
Pub. in Proceedings of the SPIE Conference on Effective Utilization of Optics in Quality Assurance, Arlington Heights, IL., November 14-16, 1977, v129 p9-11 1978.

Keywords: *Helium neon lasers, *Dimensional measurement, *Length, *Standards, Stabilization, Length.

The iodine stabilized helium-neon laser is the most accurate and stable standard of length that is available for general metrological use today. Although the krypton discharge lamp is still the basis for international agreements which define the meter as the length standard, the independent reproducibility of the iodine stabilized helium-neon laser has been shown to exceed that of the krypton lamp when international intercomparisons are made. Because of its superior performance, the iodine stabilized helium-neon laser is used in most national standards laboratories to realize the stand of length. A value for its wavelength which is consistent with the value for the wavelength of the krypton lamp has been agreed upon by the metrological community through consultation with the International Bureau of Weights and Measures.

*601,035*
**PB86-206372**
(Order as PB86-206364, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Ruggedness Testing - Part 1: Ignoring Interactions,**
R. C. Paule, G. Marinenko, M. Knoerdel, and W. F. Koch. 29 Aug 85, 6p
Included in Jnl. of Research of the National Bureau of Standards, v91 n1 p3-8 Jan-Feb 86.

Keywords: *Durability, *Mechanical properties, Electrodes, Mathematical models, Field tests, Design, Statistical analysis, pH, Hydrochloric acid.

A straightforward explanation of the statistical technique of ruggedness testing is presented. Efficient Plackett-Burman designs are used in ruggedness tests. These designs involve the simultaneous change of levels ofa number of variables. The designs allow the ruggedness test user to determine the effect of the separated variables on the measurement process.

*601,036*
**PB86-206380**
(Order as PB86-206364, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Ruggedness Testing - Part 2: Recognizing Interactions,**
R. C. Paule, G. Marinenko, M. Knoerdel, and W. F. Koch. 28 Aug 85, 7p
Included in Jnl. of Research of the National Bureau of Standards, v91 n1 p9-15 Jan-Feb 86.

Keywords: *Electrodes, *Durability, Test methods, Measurement, pH, Acidity, Interactions, Ruggedness.

The paper is a continuation of the preceeding article which introduced the reader to the general concepts of ruggedness testing. The current paper describes the effects of interactions on the measurement process, and presents procedures for the separation of the main effects from the two-factor interactions. The general characteristics of interactions are described in some detail. A short-cut procedure is presented for the calculations. A number of examples of glass electrode measurements of pH of dilute acid solutions are used to illustrate ruggedness testing proceudres.

*601,037*
**PB86-213006** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Summary of the Second Biennial Conference on Refrigeration for Cryogenic Sensors and Electronic Systems.**
Final rept.,
J. E. Zimmerman. 1983, 2p
Pub. in Cryogenics 23, n5 p281-282 1983.

Keywords: *Meetings, *Refrigerating, Cryogenics, Detectors, Electric equipment, Reprints.

The report is a summary of the Second Biennial Conference on Refrigeration for Cryogenic Sensors and Electronic Systems held at NASA Goodard Space Flight Center, Greenbelt, MD.

*601,038*
**PB86-214707** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Use of Back-to-Back Accelerometers as Precision Vibration Standards.**
Final rept.,
B. F. Payne. 1982, 4p
Pub. in Proceedings of International Modal Analysis Conference and Exhibit (1st), Orlando, FL., November 8-10, 1982, p212-215.

Keywords: *Accelerometers, *Calibrating, Vibration, Vibration meters, Standards.

Precision vibration measurements depend on accurate and repeatable calibration methods. Standardization of calibration test equipment and measurement techniques ensures more accurate and repeatable measurements. The use of the back-to-back accelerometer as a laboratory standard has become wide-spread. However this use has been somewhat limited because of inadequate calibration methods. Recent developments in improved calibration methods has given the back-to-back accelerometer a greater potential as an accurate, repeatable, and stable vibration standard. As a vibration standard, the back-to-back accelerometer should prove to be a valuable asset for laboratories involved in vibration measurements and vibration transducer calibrations. Recent work at NBS in this area is presented with some examples of transducer calibrations on these standards.

*601,039*
**PB86-215167** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Minimum Life Cycle Cost Heat Losses for Shallow Trench Underground Heat Distribution Systems,**
J. B. Fang. May 86, 46p NBSIR-86/3381
Sponsored by Corps of Engineers, Washington, DC., Naval Facilities Engineering Command, Alexandria, VA., and Air Force Engineering and Services Center, Tyndall AFB, FL.

Keywords: *Pipes(Tubes), *Heat loss, Thermal insulation, Heat transfer, Life cycles, Service life, *Heat pipes.

The rates of heat loss from two underground insulated pipes installed in a shallow trench were calculated using a computer program developed based on the application of the finite element method to solution of two-dimensional steady heat conduction problems. The calculated results of pipe heat loss under a specified ground temperature condition are summarized for a range of pipe insulation thickness, different sizes of shallow trench, and various pipe fluid temperatures. Methods of determining the minimum life-cycle cost heat loss and the corresponding economic insulation thickness for shallow trench heat distribution systems are presented. Life-cycle costing analysis was performed for two insulated pipes in a concrete trench to determine the cost of construction, annual energy cost associated with pipe heat loss, and yearly operating and maintenance costs.

*601,040*
**PB86-231511** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Polyvinylidene Fluoride Transducer for Dynamic Pressure Measurements.**
Final rept.,
E. R. Lemar, J. W. Forbes, D. G. Tasker, and A. J. Bur. 1985, 6p
Pub. in Proceedings of Topical Conference on Shock Waves in Condensed Matter, Spokane, WA., July 22-25, 1985, p1-6.

Keywords: *Pressure sensors, Pressure gages, Piezoelectric transducers, Vinylidene fluoride polymers.

A number of light gas gun experiments have been performed to measure the charge output of electrically poled polyvinylidene fluoride (PVDF) as a function of uniaxial strain. The .05 mm thick gage package was epoxied between two 1.27 thick plexiglas discs. The plexiglas was impacted by 6061 T6 aluminum projectiles resulting in pressures ranging from 0 to 15 kbars. The charge output from the gage was observed to have an initial step with rise time of 0.1 microsec. Nonlinear response at high pressures is observed.

*601,041*
**PB86-232295** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Applications of Radiation Thermometry.**
Final rept.,
J. C. Richmond, and D. P. DeWitt. 1986, 171p
Pub. in Proceedings of Symposium on Applications of Radiation Thermometry, Gaithersburg, MD., May 8, 1984, ASTM Special Publication 895 - Applications of Radiation Thermometry, 171p 1986.

Keywords: *Temperature measurement, Temperature measuring instruments, Temperature control, Fiber optics, Calibrating, Laboratories, Glass, Crystal growth, Steels, Reheating, Ovens, Welding, Pyrometers, Semiconductors, Imaging techniques.

Contents: Radiation thermometry--the measurement problem; Methods of calibration at a national laboratory; Establishing a calibration laboratory for industrial radiation thermometry; Radiation thermometry--status and trends; Mold temperature measurement for glass-pressing processes; Use of infrared radiation thermometers for temperature control of plastic and paper webs in electric infrared ovens; Radiation thermometry for semiconductor crystal growing furnaces; Thermal imaging systems for measuring temperature distribution; A review of temperature measurement in the steel reheat furnace; Closed-loop temperature control for high-frequency electric-resistance tube and pipe welding mills; Recent advances and research activities in Japan; Fiber-optic thermometry; Panel discussion.

*601,042*
**PB86-232444** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Measuring Linewidths with an Optical Microscope.**
Final rept.,
C. P. Kirk, and D. Nyyssonen. 1986, 12p
Pub. in Test and Measurement World, p68-79 Jan 86.

Keywords: *Line width, *Optical measurement, Reprints.

## General

No abstract available.

*601,043*
**PB86-238813** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of the Director.
**Measurement Accuracy - RF to Optical.**
Final rept.,
E. Ambler. Jan 86, 2p
Sponsored by Institute of Electrical and Electronics Engineers, Inc., Washington, DC.
Pub. in Proceedings of Institute of Electrical and Electronics Engineers 74, n1 p7-8 Jan 86.

Keywords: *Metrology, Measurement, Calibrating, Microwaves, Optical communication.

Various developments in microwave and optical metrology that have been stimulated by the needs of satellite and optical fiber telecommunications are discussed. A few recent examples of the symbiosis of science, technology, and metrology in the microwave and optical fields are noted. Meeting the challenge of providing calibration support to the new automated measurement systems is seen to require a high degree of cooperation among government, industry, and the universities.

*601,044*
**PB86-241932** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiation Gauging.**
Final rept.,
J. H. Hubbell. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v6 p4040-4042 1986.

Keywords: *Measuring instruments, X rays, Gamma rays, Electrons, Neutrons, Radiometry, Reprints.

Gauges employing penetrating radiation such as x- or gamma-rays, electrons, or neutrons, are discussed. Such a gauge consists of a radiation source and a radiation sensor which detects the fraction of source radiation transmitted by the examined material, or in some applications detects secondary radiation such as scattered or fluorescence photons resulting from interactions of the source-radiation with atoms of the material. Some examples of currently-used radiation gauges are mentioned.

*601,045*
**PB86-241957** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Ultrasonic Reference Blocks.**
Final rept.,
D. G. Eitzen, and G. V. Blessing. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v7 p5182-5186 1986.

Keywords: *Standards, Nondestructive tests, Ultrasonic tests, Reprints, *Reference blocks.

The article describes the functions of ultrasonic reference artifacts as a tool for setting ultrasonic test sensitivity, as an aid in interpreting signals and as a tool for classifying test parts. The design considerations of reference blocks relating to material, outer geometry, and reflector geometry are described. The most common reference blocks, the IIW Block and the ASTM E-127 Block, are described. References for additional information are listed.

*601,046*
**PB86-244159** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**International System of Units (SI).**
Special pub.,
D. T. Goldman, and R. J. Bell. Jul 86, 61p NBS/SP-330
Supersedes PB82-154584. Also available from Supt. of Docs as SN003--003-02739-1. Prepared in cooperation with National Physical Lab., Teddington (England).

Keywords: *Metric system, Units of measurement, Primary standards, Translations, *Foreign technology, *International system of units.

The booklet is the United States edition of the English translation of the fifth edition of 'Le Systeme International d'Unites (SI),' the definitive publication in the French language issued in 1985 by the International Bureau of Weights and Measures (BIPM). This U.S. edition, which conforms in substance with the British edition that follows the French text in the BIPM document is the result of a joint effort by the National Bureau of Standards(NBS) of the United States and the National Physical Laboratory (NPL) in the United Kingdom.

*601,047*
**PB86-246162** PC **A10**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Office of Physical Measurement Services.
**NBS (National Bureau of Standards) Calibration Services Users Guide 1986-88 Edition,**
G. A. Uriano, E. L. Garner, R. K. Kirby, and W. P. Reed. Jul 86, 208p NBS/SP-250
Supersedes PB83-151662. Also available from Supt. of Docs as SN003-003-02749-9.Color illustrations reproduced in black and white.

Keywords: *Calibrating, *Measurement, Standards, Services, National Bureau of Standards.

The NBS Calibration Service Users Guide provides detailed descriptions of the currently available NBS calibration services, special test services, and measurement assurance programs. The document is a revised edition of NBS Special Publication 250. It describes the NBS services available as of the second quarter of 1986 and reflects a number of important changes since the 1982 edition was published. A detailed description is given of each measurement service. A new numbering system is used to uniquely identify each of the services. Addendum I to this document is a cross-reference index that links the new NBS test numbers to those used previously to identify the services. Also cited are a large number of NBS technical experts (including addresses and telephone numbers) who may be contacted for further information concerning services or measurement problems. Future editions will be published periodically as NBS services change. The document also presents a detailed description of a number of Measurement Assurance Program (MAP) services.

*601,048*
**PB87-103313** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Tensile Properties of Pleated Synthetic Rope,**
S. G. Fattal. Sep 86, 44p NBSIR-86/3375
Sponsored by Aberdeen Proving Ground, MD.

Keywords: *Rope, Nylon fibers, Tensile properties, Breaking load, Elongation.

Pleated nylon ropes of two sizes and approximately the same length were tensioned to rupture in a universal testing machine. Several of the ropes were tested at room temperature. The others were subjected to specified high and low temperatures before testing. Deformation measurements of all the specimens were recorded while testing was in progress. The results were used to evaluate the breaking strength, ultimate elongation, and load-deformation properties, and to develop criteria for possible application in the recovery of mired vehicles.

*601,049*
**PB87-108429** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Comparison of Three Types of Pulse Tube Refrigerators: New Methods for Reaching 60 K.**
Final rept.,
R. Radebaugh, J. Zimmerman, D. R. Smith, and B. Louie. 1986, 11p
Contract NASA-A-14746-C
Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center.
Pub. in Advances in Cryogenic Engineering 31, p779-789 1986.

Keywords: *Refrigerators, Cryogenics, Reprints, *Pulse tube refrigerators.

The paper compares the three types with each other and with common refrigerators such as Joule-Thomson and Stirling refrigerators. An apparatus is described which can measure the intrinsic behavior of the different types from temperatures of about 30 K to 300 K. Overall cycle efficiency as well as sources of loss such as conduction and regenerator ineffectiveness are discussed and the advantages of various phase shifting techniques to increase refrigeration capacity are compared.

*601,050*
**PB87-111688** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Fitness-for-Service Assessment of Pipeline Girth Welds with Emphasis on Nondestructive Inspection.**
Final rept.,
R. P. Reed, and R. E. Schramm. 1986, 7p
Sponsored by Department of Transportation, Washington, DC. Materials Transportation Bureau, Naval Sea Systems Command, Washington, DC., and Welding Research Council, New York.
Pub. in Proceedings of International Conference and Exposition on Fatigue, Corrosion Cracking, Fracture Mechanics and Failure Analysis, Salt Lake City, UT., December 2-6, 1985, p255-263 1986.

Keywords: *Welded joints, Pipelines, Nondestructive tests, Inspection.

A review of fitness-for-service assessment of pipeline girth welds is presented. The U.S., British, Japanese, and Canadian approaches are summarized and compared in terms of allowable flaw sizes. Included is an in-depth discussion of nondestructive inspection of girth welds, using electromagnetic-acoustic transducers (EMATs), EMATs have great potential as an inspection tool for sharp flaws, those flaws that most affect weld structural integrity.

*601,051*
**PB87-111837** PC **A11**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Impact-Echo: A Method for Flaw Detection In Concrete Using Transient Stress Waves,**
M. Sansalone, and N. J. Carino. Sep 86, 237p
NBSIR-86/3452
Supersedes PB87-104444.

Keywords: *Nondestructive tests, *Concretes, Finite element analysis, Greens function, Stress waves, Plates(Structural members), *Flaw detection.

The report covers a nondestructive test method for heterogeneous solids. Analytical, numerical, and laboratory studies of transient stress wave propagation in plain plates and in plates containing flaws are presented. The test method involves introducing transient stress waves into a test object by mechanical point impact and monitoring reflections of the waves from internal defects and external boundaries using a point receiver.

*601,052*
**PB87-128195** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Electrochemical Noise as an Indicator of Anaerobic Corrosion.**
Final rept.,
W. P. Iverson, and L. Heverly. 1986, 13p
Pub. in American Society for Testing and Materials STP 908--Corrosion Monitoring in Industrial Plants Using Nondestructive Testing and Electrochemical Methods, p459-471 1986.

Keywords: *Pipelines, *Corrosion, *Anaerobic bacteria, Reprints, Microbial corrosion, Desulfovibrio, Electrochemical noise, Sulfate reducing bacteria.

Anaerobic (bacterial) corrosion is an important cause of failures of underground structures, such as pipelines. Pipeline failures could be prevented if better methods for determining the presence and location of areas of bacterial corrosion existed. A technique was developed which permits the detection and recording of rapid potential fluctuations (noise) produced in a corroding metal. It is believed that the noise is mainly caused by the breaking of protective films on the metal surface. Anaerobic bacterial corrosion also produces a type of noise, probably due to the breaking of iron sulfide films. Preliminary evidence indicates that detection and production of the noise on pipelines may offer promise in locating areas of microbial corrosion as well as other types of corrosion. Differences in the type of noise signal could enable differentiation between biological and nonbiological corrosion.

*601,053*
**PB87-131314** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

**Measurements of the Efficiency and Refrigeration Power of Pulse-Tube Refrigerators,**
S. Herrmann, and R. Radebaugh. Sep 86, 54p NBS/TN-1301
Also available from Supt. of Docs as SN003-003-02771-5. Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center.

Keywords: *Refrigerators, Cryogenics, *Cryocoolers, Regenerative cooling.

Pulse-tube or thermoacoustic refrigerators have the potential for high reliability since they require only one moving part--an oscillating piston or diaphragm at room temperature. If a tube is closed at one end and connected to a pressure wave generator at the open end, and if the phase angle between mass flow and pressure is shifted from 90 deg, then refrigeration occurs at the open end. The shift in phase angle can be realized by thermal relaxation between the gas and the tube walls or by an orifice at the closed end. A low temperature of 60 K using helium gas in a one stage orifice pulse tube has been achieved at NBS. The report describes the first measurements of the efficiency, refrigeration power, and refrigeration power per unit mass flow, for three pulse-tube refrigerators. Three tube sizes, differing in length and diameter, were studied over a frequency range of 3 to 11.5 Hz. Cooling efficiencies as high as 90% of the Carnot efficiency were obtained when compressor and regenerator losses are neglected.

# LIBRARY & INFORMATION SCIENCES

## Information Systems

*601,054*

**PB86-154002** CP **T02**
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Codes for Named Populated Places, Primary County Divisions, and Other Locational Entities of the United States (FIPS PUB 55), 8th Update.**
Data file,
H. Tom. Feb 86, mag tape FIPS PUB 55, NBS/DF/MT-86/003
Supersedes PB85-152312.
Source tape is in the EBCDIC or ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. Call NTIS Computer Products if you have questions.

Keywords: *Data file, *Coding, *United States, Urban areas, Rural areas, Municipalities, Communities, States(United States), Magnetic tapes, *Federal information processing standards, *Geocoding, Standard metropolitan statistical areas, Counties, ZIP codes.

The eighth update of the Federal Information Processing Standard (FIPS) 55 data file provides a two-character State code and five-character numeric place code to uniquely identify each listed entity. Areas of the United States covered are the fifty States, the District of Columbia, and all outlying territories with significant self-administration. An exhaustive list is carried of incorporated places, census designated places (CDP's), primary county divisions (such as townships, New England towns, and census county divisions), recognized Indian reservations and Alaska Native villages, and counties. The listing also includes unincorporated places, military bases, National parks, airports, and ground transportation points.

*601,055*

**PB86-212982** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Data Base Management Systems, Part 1: A Quick Overview.**
Final rept.,
D. B. Neumann. 1985, 13p
Pub. in Nonbibliographic Data Banks in Science and Technology, p139-151 1985.

Keywords: *Chemistry, Data processing, Reprints, *Data base management systems, *Numeric data bases, Data bases, Data banks.

An overview of data-base management systems (DBMS's) is presented. Examples are drawn primarily from a single case: a two-level network-type system. The terminology of data-base systems, their access methods, and their structures are introduced.

*601,056*

**PB86-212990** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Data Base Management Systems. Part 2. An Application to Scientific Technical Data and Its Associated Bibliographic Data.**
Final rept.,
D. B. Neumann. 1985, 13p
Pub. in Nonbibliographic Data Banks in Science and Technology, p153-165 1985.

Keywords: *Thermochemistry, Chemistry, Data processing, Networks, Bibliographies, Reprints, *Data base management systems, Numeric data bases, Data structures, Data bases, Hewlett-Packard computers.

A data-base management system (DBMS) permitting only a two-level network schema has been applied to a relatively complex data base. Such an application to a thermochemical data base is described here. The test case studied was the Hewlett-Packard IMAGE/1000 DBMS. The logical and physical structure of the thermochemical data base is described. Methods used to overcome the limitations of the two-level network DBMS are also discussed.

*601,057*

**PB87-120036** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Information Systems Engineering Div.
**Database Conversions Demand Common Standards for Data Structure.**
Final rept.,
L. J. Gallagher. 1985, 6p
Pub. in Data Management 23, n1 p22 and p24-28 Jan 85.

Keywords: *Standards, *Conversion, *Data processing, Programming languages, Specifications, Translations, Information systems, Decentralization, Work, Reprints, *Data bases, *Data structures, *Distributed processing, *Applications programs(Computers).

The proliferation of small and medium sized computers has made it possible to decentralize the data processing work load into a number of smaller distributed tasks. With this decentralization, there is an increasing need to translate data and application programs from one computer processing environment to another. To serve this need there has been welcome progress in the specification of national and international standards for data definition, data manipulation, and data interchange. The paper discusses standard specifications for database languages recently completed by technical committee X3H2 of the American National Standards Institute and for data interchange forms recently adopted by the International Organization for Standardization. It shows by example how a complete database application can be transported or shared in a standard manner among different computer processing environments.

*601,058*

**PB87-136677** PC **A07**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
**Materials Information for Science and Technology (MIST): Project Overview.**
Final rept.,
W. Grattidge, J. Westbrook, J. McCarthy, C. Northrup, and J. Rumble. Nov 86, 132p NBS/SP-726
Also available from Supt. of Docs as SN003-003-02780-4. Library of Congress catalog card no. 86-600590. Prepared in cooperation with Sci-Tech Knowledge Systems, Inc., Scotia, NY., Lawrence Berkeley Lab., CA., and Sandia National Labs., Albuquerque, NM.

Keywords: *Materials, *Information systems, Engineering, Data processing, Computer networks, *Data base management, *Data bases, *MIST data base, *Science and Technology development, Numeric data base, Access, Department of Energy, National Bureau of Standards, Distributed computer systems.

The report documents the initial phases of the MIST database, which is a demonstration project jointly supported by the Department of Energy and the National Bureau of Standards. The purpose of the Materials Information for Science and Technology (MIST) is to demonstrate the power and utility of computer access to materials property data. The initial goals include: to exercise the concept of a computer network of materials databases and to build a demonstration of such a system in a way as to be suitable for use as the core of operational systems in the future. Phases I and II are described in detail. In addition, a discussion is given of the expected usage of the databases.

## Marketing & User Services

*601,059*

**PB86-202116** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
**Information Resource Centers - Organizing to Serve End Users.**
Final rept.,
T. N. Pyke. 1983, 4p
Pub. in Proceedings of the IEEE (Institute of Electrical and Electronics Engineers, Inc.) Computer Society International Conference (27th) COMPCON 83 Fall: Delivering Computer Power to End Users, Arlington, VA., September 25-29, 1983, p22-25.

Keywords: *Information centers, Organizations, Microcomputers, Access, Systems engineering, Services, *Mainframe computers, *User needs, End use.

The paper summarizes the motivation for and issues associated with organizing to support end user direct access to computing resources. A combination of information center functions to provide access to large mainframes and support to end users in their access to microcomputers is included. Various issues are identified and discussed that will help organizations develop supporting organizational structures for end user computing.

## Operations & Planning

*601,060*

**PB86-191152** PC **A12**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
**Data Administration Workshop Proceedings,**
F. E. Spielman. Feb 86, 256p NBSIR-86/3324
Proceedings of a workshop held at Gaithersburg, Maryland on March 27-28, 1985.

Keywords: *Meetings, Costs, Planning, Tools, Standards, *Data administration.

The Special Publication constitutes the proceedings of a two-day workshop on Data Administration, held at the National Bureau of Standards, Gaithersburg, Maryland, on March 27-28, 1985. The workshop was sponsored by the National Bureau of Standards under the auspices of the Federal Data Management Users' Group (FEDMUG). The purpose of the workshop was to provide a forum for Federal, State, and local government Program Managers, Information Resource Managers, Data Processing Managers, and Data Administrators to hear nationally prominent speakers and to discuss and share data administration ideas and experiences.

*601,061*

**PB86-247582** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Information Resources and Services Div.

## Operations & Planning

**NBS (National Bureau of Standards) Research Information Center Handbook for NBS Staff (Fourth Edition),**
L. S. Maruyama. Aug 86, 69p NBSIR-86/3394

Keywords: *Information centers, Libraries, Handbooks, Services, Resources, National Bureau of Standards, Federal libraries.

The directory describes the information resources and services of the National Bureau of Standards Research Information Center.

### Reference Materials

*601,062*
**PB86-191871** PC **A08**/MF **A01**
Toth (R.B.) Associates, McLean, VA.
**Federal Government Certification Programs for Products and Services.**
Final rept.,
R. B. Toth. Apr 86, 160p NBS/SP-714
Also available from Supt. of Docs as SN003-003-02719-7. Library of Congress catalog card no. 86-600516. Sponsored by National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.

Keywords: *Directories, *National Government, *Services, Regulations, Standards, Inspection, Industries, Data bases, *Certification, *Commodities.

The directory presents information on 61 U.S. Government certification programs for products and services. Entries describe the scope and nature of each certification program, testing and inspection practices, standards used, methods of identification and enforcement, reciprocal recognition or acceptance of certification, and other relevant details. The directory is part of an ongoing NBS effort to establish and maintain a comprehensive database on standards, regulations, certification programs and related information. The material has been compiled to meet the needs of government, industry, and the public for information on U.S. Government certification programs in accordance with the requirements of the U.S. Trade Agreements Act of 1979.

*601,063*
**PB86-193083** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
**National Standard Reference Data System of the United States.**
Final rept.,
D. R. Lide. 1984, 4p
Pub. in Computer Physics Communications 33, n1-3 p207-210 Aug/Sep 84.

Keywords: *Standards, *Physics, Information centers, United States, Evaluation, Reprints, *Standard reference data.

The operation of the National Standard Reference Data program is described. A list of data centers of interest to the physics community is given.

*601,064*
**PB86-201290** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Center for Electronics and Electrical Engineering Technical Publication Announcements Covering Center Programs, July to September 1985 with 1986 CEEE Events Calendar,**
E. J. Walters. Apr 86, 22p NBSIR-86/3366

Keywords: *Bibliographies, *Electronics, *Electrical engineering, National Bureau of Standards.

This is the sixth issue of a quarterly publication providing information on the technical work of the National Bureau of Standards Center for Electronics and Electrical Engineering. The issue of the CEEE Technical Publication Announcements covers the third quarter of calendar year 1985.

*601,065*
**PB86-215142** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Public Information Div.
**NBS (National Bureau of Standards) Research Reports, May 1986.**
May 86, 34p NBS/SP-680/5
See also PB86-129707. Library of Congress catalog card no. 86-600534.

Keywords: *Research projects, Surface roughness, Polymers, Standards, Commerce, International trade, Algae, Diets, Stellar magnetic fields, Image processing, Flare stars, US NBS.

Contents:
- Research update;
- A perspective on the future of NBS;
- Surface roughness monitor for advanced manufacturing developed;
- Artificial vision device performs high-speed processing of images;
- Taking the 'guesswork' out of making polymer blends;
- Standards and global trade--a government perspective;
- Counterfeit chlorophyll, artificial algae-the perfect energy device;
- Burgers, fries, pizza pies--all part of massive study of worldwide diets;
- JILA astronomers first to detect magnetic fields on a flare star;
- New publications;
- Conference calendar.

*601,066*
**PB86-232006** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Center for Electronics and Electrical Engineering Technical Progress Bulletin Covering Center Programs, October-December 1985 with 1986 CEEE Events Calendar,**
E. J. Walters. Jun 86, 36p NBSIR-86/3344/2
See also PB85-191393.

Keywords: *Electronics, *Electrical engineering, *Bibliographies, National Bureau of Standards.

This is the thirteenth issue of a quarterly publication providing information on the technical work of the National Bureau of Standards Center for Electronics and Electrical Engineering. The issue of the CEEE Technical Progress Bulletin covers the fourth quarter of calendar year 1985. Abstracts are provided by technical area for both published papers and papers approved by NBS for publication.

*601,067*
**PB86-237260** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Public Information Div.
**NBS (National Bureau of Standards) Research Reports, February 1985,**
S. Shaffer. Feb 85, 36p NBS/SP-680/2
See also PB85-127421. Library of Congress catalog card no. 84-601166.

Keywords: *Research projects, *Technology assessment, Computer networks, Earthquakes, Radiation, Metal industry, Alloys, National Bureau of Standards.

This report covers the following topics: Research update; NBS and steel producers join in high-risk research; Metals-processing technology for the future; Diagrams for designing alloys; Radiation: Keeping the genie under control; Tools and technology for the building industry; New facility used to simulate earthquake forces; Welcome to the new computer age: The era of networks; NBS perspective on open systems interconnection; NBS adds credibility to energy-related inventions; New publications, and Conference calendar.

*601,068*
**PB86-247616** PC **A07**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Information Resources and Services Div.
**Data Bases Available at the National Bureau of Standards Research Information Center (Fifth Edition),**
D. Cunningham. Jul 86, 135p NBSIR-86/3428
See also 3rd edition, PB83-155986.

Keywords: *Information systems, *Directories, Information centers, Indexes(Documentation), *Bibliographic data bases, *Data bases, National Bureau of Standards.

An alphabetical listing of data bases available online at the National Bureau of Standards (NBS) Research Information Center is listed by either acronym or full title of the data base. Other additional information includes description of the data base, period of coverage, producer(s), corresponding hard copy, principal sources and vendors. A general subject index and a cross reference index to the data bases are also supplied.

*601,069*
**PB87-106720** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
**National Bureau of Standards. Journal of Research of the**
Final rept.,
C. Eisenhart. 1985, 6p
Pub. in Encyclopedia of Statistical Sciences v6, p150-155 1985.

Keywords: *Periodicals, Research, National Bureau of Standards.

The founding of the Bureau, its primary mission and expanded scope through subsequent legislation. History of its Journal of Research, with particular attention to papers published from 1947 through 1982 that contain material on probability theory, statistical theory and methodology, or applications thereof of potential interest to statisticians and teachers of statistics.

*601,070*
**PB87-129011** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
**CODATA Role in International and Interdisciplinary Cooperation.**
Final rept.,
D. R. Lide. 1984, 2p
Pub. in Computer Physics Communications 33, n1-3 p205-206 Aug/Sep 84.

Keywords: Scientific societies, Experimental data, Data processing, Standards, Distributing, Reprints, *Scientific data, *Interdisciplinary cooperation, International cooperation, Data compilation, Disseminating, References(Standards).

International cooperation in the compilation of scientific data is briefly reviewed. The organization and administrative structure of CODATA are described. Several types of CODATA activities are summarized.

### General

*601,071*
**PB86-231487** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Information Resources and Services Div.
**Federal Government Libraries and Information Centers,**
P. W. Berger. 1986, 13p
Pub. in Education for Professional Librarians, Chapter 8, p141-153 1986.

Keywords: *Librarians, *Technical information specialists, Education, Standards, Reprints, *Federal librarians, Federal government.

The report is a chapter in a book edited by Herbert White. The chapter reviews the development and applications of educational standards for librarians and technical information specialists in the federal government since 1966. Some conspicuous developmental and application failures are discussed as well, and a possible hedge against future disasters is suggested.

*601,072*
**PB87-140604** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
**Cost Comparison of Selected Alternatives for Preserving Historic Pension Files.**
Final rept.,
R. E. Schofer. Jul 86, 59p NBSIR-86/3335
Sponsored by National Archives and Records Administration, Washington, DC.

Keywords: *Records management, *Cost estimates, Systems analysis, Archives, Labor estimates, Microfilm, Preservation, Services, Historic pension files.

The report describes the results of a cost study of three selected alternatives for preserving the historic pension files. The three alternatives evaluated comprise three levels of technology: Hand retrieval of original paper documents; Hand retrieval of microfiche copies of the original documents; and Automatic retrieval of microfiche copies. Results indicate that the microcopy alternatives substantially reduce storage space requirements and the labor cost of providing reference service. The automated-retrieval-alternative reduction in labor cost is very substantial. However, the extremely high cost of converting the files to microfiche more than cancels out the savings in both space and operating costs, except under very high reference usage. Improving the storage environment and continuing reference service with the original documents is an attractive alternative. At current usage rates, each file is requested, on the average, every 65 years. At these rates, preservation experts do not expect the documents to deteriorate from reference usage.

# MANUFACTURING TECHNOLOGY

## Computer Aided Design (CAD)

*601,073*
**PB86-209897** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**IGES (Initial Graphics Exchange Specification), a Key Interface Specification for CAD/CAM Systems Integration.**
Final rept.,
B. Smith, and J. Wellington. 1984, 8p
Pub. in Proceedings of Annual Conference and Exposition - National Computer Graphics Association, Computer Graphics '84 (5th), Anaheim, CA., May 13-17, 1984, p548-555.

Keywords: *Computer graphics, *Data displays, Standardization, Specifications, *Computer aided design, *Computer aided manufacturing, Data exchange, Vendors.

The Initial Graphics Exchange Specification (IGES) program has focused the efforts of 52 companies on the development and documentation of a means of graphics database exchange among present day CAD/CAM systems. The project's brief history has seen the evolution of the Specification into preliminary industrial usage marked by public demonstrations of vendor capability, mandatory requests in procurement actions, and a formalization into an American National Standard in September 1981. Recent events have demonstrated intersystem data exchange among seven vendor systems with a total of 30 vendors committing to offer IGES capability. A full range of documentation supports the IGES project and the recently approved IGES Version 2.0 of the Specification.

*601,074*
**PB87-134334** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Current Ability of the Architecture, Engineering, and Construction Industry to Exchange CAD (Computer-Aided Design) Data Sets Digitally.**
Final rept.,
M. E. Palmer. Oct 86, 38p NBSIR-86/3476
Contract N68305-86-W-R60132
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Computer graphics, *Constructure industry, Architecture, Engineering, Standards, Guidelines, Specifications, *Computer aided design, *Data exchange, *Translators, Digital data, Software tools, Computer program documentation.

The current ability of the AEC industry to exchange CAD information digitally has been assessed through discussions with AEC CAD users and consultants, site visits to CAD installations, and reviews of CAD software and translator documentation. The principal conclusions and recommendations of the report are as follows: (1) In order to take fully advantage of CAD and to maximize the utilization of digital project information, this industry requires a dependable method for the digital data exchange; (2) The current generation of translator tools is inadequate for comprehensive AEC CAD operations, incomplete translators, insufficient documentation, and differing interpretations of specifications have prevented accurate and complete data set exchanges and; (3) There is a critical need for a public program to validate translator software, to identify problems in current implementations, and to develop guidelines for the use of computer data exchange standards.

## Computer Aided Manufacturing (CAM)

*601,075*
**PB86-199759** PC **A22**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Initial Graphics Exchange Specification (IGES), Version 3.0.**
Rept. for Jan 83-Dec 85,
B. Smith, and J. Wellington. Apr 86, 525p NBSIR-86/3359
See also PB83-137448. Errata sheet inserted.

Keywords: *Computer graphics, Specifications, *Computer aided manufacturing, *File maintenance, *Data interchange, Data structures, Computer aided design.

The document contains Version 3.0 of the Initial Graphics Exchange Specification, a defined format for the creation of a file which enables data found in today's commercially available CAD/CAM systems to be exchanged or archived. IGES, Version 1.0, published as NBSIR 80-1978 (R) in January 1980, consisted of entity definitions for geometry, drafting and structural information. Definition entities were provided as a means of expanding the utility of IGES. Version 3.0 further refines the concept and offers increased capability in both geometry and non-geometry data exchange. The applications of printed wiring boards and finite element models are well supported in addition to enhancements for mechanical products.

*601,076*
**PB86-232402** PC **A04**/MF **A01**
Michigan Univ., Ann Arbor. Graduate School of Business Administration.
**Simulation Model for the Automatic Turning Station at the Automated Manufacturing Research Facility,**
N. Raman, F. B. Talbot, and R. V. Rachamadugu.
Mar 86, 62p NBS/GCR-86/513
See also PB86-231305. Sponsored by National Bureau of Standards, Gaithersburg, MD.

Keywords: *Turning(Machining), *Computerized simulation, Automation, Computer programs, Scheduling, Real time operations, Robots.

The report is part of the ongoing project on the real-time scheduling of the Automated Manufacturing Research Facility at the National Bureau of Standards in Gaithersburg, Maryland. In an earlier paper, Rachamadugu, Raman and Talbot (1986) reported on the performance of the Automatic Turning Station (ATS) under nine dispatching procedures and presented a simulation-based evaluation of these procedures. The paper presents the simulation model used in the study mentioned above and presents the steps required to execute the model.

*601,077*
**PB86-238821** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Control System for an Automated Manufacturing Research Facility.**
Final rept.,
J. S. Albus, A. J. Barbera, and M. L. Fitzgerald. 1984, 17p
Sponsored by Society of Mfg. Engineers, Dearborn, MI.
Pub. in Proceedings of Conference on Robots 8, Detroit, MI., June 4-7, 1984, Volume 2: Future Considerations, p13.28-13.44.

Keywords: *Control equipment, *Automation, Robots, Real time operations, *Computer aided manufacturing.

A hierarchical architecture for real-time planning and control has been implemented in the first Cell of an Automated Manufacturing Research Facility at the National Bureau of Standards. Three workstations (A horizontal milling, a turning, and a materials handling workstation) have been implemented. The horizontal and the turning workstations have robots, and the horizontal has a 6-D robot vision system interfaced with a RCS (Real-time Control System) robot controller. A communications network, a distributed data base and a simulator/emulator have also been implemented.

*601,078*
**PB87-103263** PC **A10**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.
**Survey of Flexible Manufacturing Systems Implementations,**
W. P. Darrow. Jul 86, 203p NBSIR-86/3413

Keywords: *Surveys, *Flexible manufacturing systems, *Computer aided manufacturing.

The report presents descriptive data on three hundred manufacturing facilities that are using computer integrated manufacturing (CIM) techniques to machine component parts for commercial, industrial, and military products. Of these, 258 were categorized as Flexible Manufacturing Systems (FMS). Key descriptive statistics were gathered for each system. The data is organized into records by the user's country, company, and geographic location. Each record is made up of 24 fields that describe the facility, the product, and the operating parameters, as well as providing a reference to the source(s) of information.

*601,079*
**PB87-107363** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Emulation as a Design Tool in the Development of Real-Time Control Systems.**
Final rept.,
H. M. Bloom, C. M. Furlani, and A. J. Barbera. 1984, 10p
Pub. in Proceedings of 1984 Winter Simulation Conference, Dallas, TX., November 28-30, 1984, p627-636.

Keywords: *Automation, Real time operations, Control equipment, Robots, *Computer aided manufacturing.

A major facility for manufacturing research is being established at the National Bureau of Standards. The Automated Manufacturing Research Facility (AMRF) will provide a testbed where measurement research of computer integrated manufacturing systems can be performed. The control architecture of the facility is based on a sensory-interactive modular hierarchical feedback system. Each module is represented as a finite state machine that interacts through a shared time-sliced common-memory where command, feedback and database information is stored. A hierarchical control system emulator (HCSE) has been developed that allows the system to be designed and tested before the implementation on the actual hardware. The HCSE has been successfully used in the AMRF project as a design management tool where the entire specification of the control software is available and as a testing aid that allows for a given module such as a robot control system to interact with the emulator when the other AMRF hardware is unavailable.

*601,080*
**PB87-108536** PC **A21**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD.
**Real-Time Optimization in Automated Manufacturing Facilities. Proceedings of a Symposium Held at the National Bureau of Standards, Gaithersburg, Maryland, January 21-22, 1986.**
Final rept.,
R. H. F. Jackson, and A. W. T. Jones. Sep 86, 487p NBS/SP-724
Also available from Supt. of Docs as SN003-003-02759-6. Library of Congress catalog card no. 86-600580. Sponsored by Department of the Navy, Washington, DC.

Keywords: *Meetings, *Automation, Real time operations, Optimization, Scheduling, Production control, *Computer aided manufacturing, *Flexible manufacturing systems.

The Symposium on Real-Time Optimization in Automated Manufacturing Facilities was held at the Nation-

al Bureau of Standards, Gaithersburg, Maryland, January 21-22, 1986. It was jointly sponsored by the Center for Manufacturing Engineering (with funds obtained from the Navy Manufacturing Technology Program) and the Center for Applied Mathematics. It was designed to bring together those who design and test optimization procedures for solving planning, scheduling, and routing problems with those who must use these procedures in a real-time manufacturing environment.

*601,081*
**PB87-129029** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Real-Time Error Compensation System for a Computerized Numerical Control Turning Center.**
Final rept.,
M. A. Donmez, K. Lee, C. R. Liu, and M. M. Barash. 1986, 8p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) International Conference on Robotics and Automation, San Francisco, CA., April 7-10, 1986, 8p.

Keywords: *Turning(Machining), *Numerical control, *Machine tools, Detectors, Microcomputers, Interfaces, *Real time system, *Error correcting devices, *Computerized control systems, Data analysis, High level language, PLM programming language, Computer software.

A real-time compensation scheme for geometric and thermally-induced errors of a computerized numerical control (CNC) turning center is described. The compensation system predicts these errors using a combination of data taken from various sensors on the machine tool and previously established relationships (transfer functions). The system translates these errors into servo counts and injects them into the control loops of the machine tool controller in real-time. A single-board microcomputer interfaced to the machine tool controller and the sensors is the workhorse of the system. The system control software written in PLM, a high level programming language, is modular, flexible, and easily maintainable.

*601,082*
**PB87-131850** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Finite Element Analysis of Flexible Fixturing System.**
Final rept.,
J. D. Lee, and L. S. Haynes. 1986, 6p
Pub. in Proceedings of Japan-USA Symposium on Flexible Automation, Osaka (Japan), July 14-18 1986, p579-584.

Keywords: *Fixtures, *Machining, Finite element analysis, Computer graphics, Automation, *Computer aided design, *Computer aided manufacturing.

A computer system has been developed for the analysis and design of fixtures. The software can lead the designer to the optimal design of the fixturing system which minimizes the total work done on the workpart, the fixturing force, the deformation index, or the maximum effective stress. The workpart is modelled as a linear isotropic elastic solid. The machining forces are simulated by specifying applied forces acting on part of the surface of the workpart. The fixturing system consists of a number of fixture elements, each in contact with the workpart with specified location and area of contact. At the interface of contact, Coulomb's law of friction is employed. The boundary conditions at the interface of contact are treated exactly. The computer software system is composed of a finite element program and computer graphic program which displays the undeformed and deformed workpart with hidden lines removed. Three sample problems have been solved and the numerical results are presented in the paper.

*601,083*
**PB87-134706** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Cell Control System for the AMRF (Automated Manufacturing Research Facility).**
Final rept.,
A. T. Jones, and C. R. McLean. 1984, 7p
Pub. in Proceedings of 1984 International Computers in Engineering Conference and Exhibit, Las Vegas, NV., August 12-15, 1984, p353-359.

Keywords: Real time operations, Interfaces, Command and control, Feedback control, *Control systems, *Cell control systems, *Command and control systems, *Manufacturing automation control, Database management systems, Operator command system, Network Communications system, Information Display system, Data structures, Computer applications, National Bureau of Standards.

The paper describes the Cell Control System developed for the Automated Manufacturing Research Facility using hierarchical task-decomposition and real-time sensory-interactive control techniques developed at NBS. The primary functions of the cell are to manage and coordinate the activities at all workstations and interface to the existing Operator Command System, Database Management System, Network Communications System, and Information Display System. In addition, the data structures developed for the command/feedback interfaces between control modules, the database transactions developed to perform inventory and job status updates, and the mailgram structures developed to transmit information over the current network, are outlined.

## Computer Software

*601,084*
**PB87-122826** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**DATAX: A Prototype Software for Engineering Data Evaluation and Decision Support.**
Final rept.,
J. T. Fong, R. S. Cramer, and D. F. Redmiles. 1984, 4p
Pub. in Proceedings of 1984 American Society of Mechanical Engineers Pressure Vessels and Piping Conference and Exhibition, San Antonio, TX., June 17-21, 1984, v96 p115-118.

Keywords: *Computer graphics, *Pressure vessels, Pipes(Tubes), Computer networks, Prototypes, Decision making, *Computer aided design, *DATAX programming language, *Computer aided manufacturing, Data base management systems, On-line systems, Formats, High level languages, Access methods, Computer software.

The extended abstract is for an invited presentation at an ASME symposium on 'Engineering Databases: Software for On-Line Applications', where a preliminary design of a prototype software named DATAX is presented. The research on DATAX was motivated by a recent study of an ASME task force on a need for developing new software and data format standards for engineering database development (ASME spec. pub. MPC-20, pp. 75-105, 1983). As a proposed software for specific use in data evaluation, DATAX is a Fortran-based high-level language designed to integrate six hitherto separate software: (1) data analysis and graphics, (2) database management system, (3) text formatting and report preparation, (4) user-driven, free-format, interactive creation of data file, (5) analysis and modeling, and (6) network access.

*601,085*
**PB87-122834** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**Engineering Databases: Software for On-Line Applications.**
Final rept.,
J. T. Fong. 1984, 128p
Sponsored by American Society of Mechanical Engineers, New York.
Pub. in Proceedings of 1984 American Society of Mechanical Engineers Pressure Vessels and Piping Conference and Exhibition, San Antonio, TX., June 17-21, 1984, v96 128p.

Keywords: *Mechanical engineering, *Programming languages, Pressure vessels, Pipes(Tubes), *Computer aided manufacturing, *Data bases, Computer software, On-line systems, Data base management systems, Computer aided design, Failure(Electronics).

The book is divided into 3 chapters. The first chapter contains 6 papers of which 5 are related to either some currently working on-line systems or some state-of-the-art software languages that are of direct interest to engineering database developers. The second chapter contains 3 papers and 3 extended abstracts on some new design concepts where the proposed databases are at various stages of implementation. The final chapter consists of an invited paper on the 'proprietary and liability aspects of on-line information and analysis systems,' and a preview of a panel session on 'new opportunities in software development and analysis systems,' and a preview of a panel session on 'new opportunities in software development and issues on copyrights.

## Engineering Materials

*601,086*
**PB87-128807** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Compressive Properties of Silica Aerogel at 295, 76, and 20 K.**
Final rept.,
J. M. Arvidson, and L. L. Scull. 1986, 8p
Pub. in Advances in Cryogenic Engineering Materials 32, p243-250 1986.

Keywords: *Compressive properties, *Silica gels, Modulus of elasticity, Compression tests, Compressive strength, Stress strain diagrams, Fractures, Reprints, *Silica aerogel.

Specimens of silica aerogel were tested in compression at 295, 76, and 20 K in a helium gas environment. The properties reported include Young's modulus, the proportional limit, and yield strength. Compressive stress-versus-strain curves at these temperatures are also given. A test apparatus was developed specifically to determine the compressive properties of low strength materials. To measure specimen strain a concentric, overlapping-cylinder, capacitance extensometer was developed. This frictionless device has the capability to conduct variable temperature tests at any temperature from 1.8 to 295 K. Results from the compression tests indicate that at low temperatures the material is not only stronger, but tougher. During 295-K compression tests, the samples fractured and, in some cases, crumbled. After 76- or 20-K compression tests, the specimens remained intact.

## Joining

*601,087*
**PB86-163797** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Use of Laser Microprobe Mass Analysis for Nickel Speciation in Individual Particles of Micrometer Size.**
Final rept.,
I. H. Musselman, R. W. Linton, and D. S. Simons. 1985, 5p
Pub. in Proceedings of Microbeam Analysis - 1985, Louisville, KY., August 5-9, 1985, p337-341.

Keywords: *Nickel, Particles, Micrometers, *Laser microprobe analysis.

Positive and negative ion spectra of micrometer-size particles of nickel metal and four nickel compounds are examined to determine the feasibility of nickel speciation by LAMMA. The four nickel compounds include nickel oxide, nickel sulfate heptahydrate, nickel sulfide, and nickel subsulfide. Diagnostic ions in both the positive and negative ion 'fingerprint' spectra distinguish nickel metal, nickel oxide, and nickel sulfate heptahydrate from nickel sulfide and nickel subsulfide. The positive and negative ion spectra of nickel sulfide and nickel subsulfide are qualitatively identical. The difficulty in differentiating the nickel sulfide and nickel subsulfide spectra using positive atomic ion intensity ratios as a reflection of compound stoichiometry is related to variations in laser power deposition and possible inhomogeneity in sample composition.

*601,088*
**PB86-232667** PC **A03**/MF **A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

**Fusion Line Shape Versus Toughness in HY-80 GMA (Gas Metal Arc) Welds,**
T. A. Siewert, R. E. Trevisan, and P. T. Purtscher.
Apr 86, 48p NBSIR-86/3043
Sponsored by David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.

Keywords: *Arc seam welds, Welded joints, Toughness, Gas metal arc welding, Steel HY-80.

The report describes the effect of the electrode weave procedure on both the fusion-line shape and toughness of reduced-gap gas metal arc (GMA welds. To study the variation in toughness, four GMA welds were produced in 25-mm-thick HY-80 plate using MIL 100S-1 electrode and following the weld procedure listed in the electrode specification, MIL-E-23765/2C. These four welds were used to compare stringer beads with various weave procedures using both manually controlled and adaptively controlled weldino systems.

*601,089*
**PB87-119137** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Production and Sizing of Uniform Two-Dimensional Flaws in Welds for NDE (Nondestructive Evaluation) Calibration.**
Final rept.,
R. E. Schramm, and T. A. Siewert. 1986, 3p
Sponsored by Naval Sea Systems Command, Washington, DC.
Pub. in Materials Evaluation 44, n9 p1136-1138 Aug 86.

Keywords: *Welded joints, *Ultrasonic tests, Nondestructive tests, Calibrating, Steels, Ultrasonic frequencies, Reprints, *Flaws.

The paper describes a procedure for the production of various uniform two-dimensional flaws for NDE calibration and their evaluation by both an electromagnetic-acoustic transducer system and metallographic sectioning.

*601,090*
**PB87-122602** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Fracture Mechanics Analysis and Critical Flaw Size Curves for Surface Flaws in Pipelines.**
Final rept.,
D. T. Read. 1986, 8p
Sponsored by Department of Transportation, Washington, DC.
Pub. in Proceedings of International Conference and Exposition on Fatigue, Corrosion Cracking, Fracture Mechanics and Failure Analysis, Salt Lake City, UT., December 2-6, 1985, p561-568 1986.

Keywords: *Standards, *Fracture tests, *Pipelines, Toughness, Stress analysis, Mechanical properties, Weld defects, Inspection, Nondestructive tests, Quality assurance, Flaw detection.

Fitness-for-purpose standards for weld inspection and flaw repair criteria offer means for rational, quantitative balance among the three critical parameters governing fracture safety; material toughness, flaw size, and applied stress. The results of fitness-for-purpose analysis can be expressed as curves dividing all possible flaws into two categories, those that must be repaired and those that may safely be left unrepaired. Such flaw tolerance curves are obtained by calculations using elastic-plastic fracture mechanics analysis. Required input for such calculations includes material strength and toughness characterization and accurate values for imposed stress.

## Manufacturing, Planning, Processing & Control

*601,091*
**PB86-203973** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Linewidth Calibration for Bright-Chromium Photomasks,**
D. Nyyssonen. May 86, 25p NBSIR-86/3357

Keywords: *Line width, Masking, Calibrating, Measurement, Chromium, Standards, Flares, Detectors, *Photomasks.

Linewidth measurement errors are introduced when an anti-reflective (AR) chromium photomask standard such as the NBS SRM 474/475 is used to calibrate an optical linewidth measurement system for subsequent measurements on another material such as bright chromium whose optical properties (index of refraction, thickness, reflectance, and edge geometry) do not match those of the calibration standard. In addition to differences in the optical properties of the materials, the magnitude of these errors varies from system to system and depends upon resolution, choice of edge-detection criterion, flare light in the optical system, and detector response. These errors are greatest when measurements are made in reflected light due to the greater sensitivity to the mismatch in optical parameters of the materials between the calibration standard (AR-chromium) and the material to be measured (bright chromium). The report, therefore, recommends use of transmitted light for linewidth measurements on photomasks and as close a match as possible between the material parameters of the calibration standard and those of the part being measured in order to ensure a realistic assessment of the accuracy and precision of subsequent measurements.

*601,092*
**PB86-212040** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**National Forum on the Future of Automated Materials Processing in U.S. Industry: The Role of Sensors. Report of a Workshop (1st) Held at Santa Barbara, California on December 16-17, 1985,**
H. T. Yolken, and R. Mehrabian. Dec 85, 79p NBSIR-86/3341
Prepared in cooperation with California Univ., Santa Barbara. Sponsored by Industrial Research Inst., New York, and Office of Science and Technology Policy, Washington, DC.

Keywords: *Material handling, *Detectors, Automation, Ceramics, Composite materials, Metals, Polymers, Optical materials.

This is the proceedings of the workshop 'A National Forum on the Future of Automated Materials Processing in U.S. Industry - The Role of Sensors'. This is the first of two workshops to be sponsored by the Industrial Research Institute and the White House Office of Science and Technology Policy, Committee on Materials Working Group on Automation of Materials Processing. The second workshop will address the other two key components required for automated materials processing, process models and artificial intelligence coupled with computer integration of the system. The objective of these workshops is to identify and assess important issues affecting the competitive position of U.S. industry related to its ability to automate production processes for basic and advanced materials and to develop approaches for improved capability through cooperative R&D and associated efforts.

*601,093*
**PB86-229945** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Electrical Measurement Technique for Estimating Proximity Effects in Electron-Beam Lithography.**
Final rept.,
D. Yen, L. W. Linholm, W. B. Glendinning, and J. F. Bass. 1983, 1p
Pub. in Jnl. of the Electrochemical Society 130, n8 p319 c1983.

Keywords: *Lithography, Electron beams, Line width, Measurement, Reprints.

An electrical test structure and test method is described for estimating the magnitude of proximity effects in electron-beam lithography. The test structure consists of van der Pauw cross resistor for measuring sheet resistance, a bridge resistor for measuring electrical linewidth, and a second bridge resistor simulating a close line-space environment for measuring electrical linewidth where proximity exposure effects from nearby patterns may be encountered. These test structures were delineated in a metal layer on a silicon wafer using electron beam exposure and wet chemical etching. Electrical measurements are compared to optical measurements. The technique provides an alternative to optical measurements for determining effective linewidth in a dense circuit environment and can be used to estimate parameters for the double Gaussian model used in proximity correction algorithm.

## Quality Control & Reliability

*601,094*
**PB86-181864** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Methodology for Statistical Control of the Anechoic Chamber Field Generation System,**
D. S. Friday. Jan 86, 20p NBSIR-85/3033

Keywords: *Anechoic chambers, *Control charts, Electromagnetic fields, Standards, *Statistical control.

The microwave anechoic chamber is a National Bureau of Standards laboratory facility in which standard electromagnetic fields are generated. The chamber enables special measurements and electromagnetic compatibility tests to be conducted on antennas and other devices. The paper is concerned with methodology for assuring that the standard field patterns generated in the chamber are repeatable. Procedures are proposed for developing a data base from measurements obtained by placing the system, which generates the fields, in certain relevant reference configurations. Methodology is presented for developing statistical control charts to monitor both the location and the scale parameters of these data over time.

*601,095*
**PB86-228616** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Release Notes for STAT2 Version 1.7: An Addendum to NBS (National Bureau of Standards) Special Publication 400-75,**
R. L. Mattis. Mar 86, 41p NBSIR-86/3333
For system on diskette, see PB86-182490. Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.

Keywords: *Computer programs, Wafers, Computer systems programs, STAT2 computer program, Automatic test equipment.

The document describes the changes which have been made in the STAT2 computer program since its documentation in NBS Special Publication 400-75, Semiconductor Measurement Technology: A FORTRAN Program for Analysis of Data from Microelectronic Test Structures, and NBS Internal Report 83-2779, Release Notes for STAT2 Version 1.31. It is assumed that the reader has these documents, and no attempt is made to review STAT2 features or operation. The changes extend the functionality and versatility of the program. More specifically, the new features added in version 1.7 include data base extension, an input data format suitable for test sites not in a periodic array, an outlier exclusion algorithm suitable for small numbers of sites, common site exclusions for related data sets, a vector map, a scatter plot, a trend chart, extended macro command file capability, and other changes. Following the description of the changes is an annotated listing of new error messages. The document and the two previous publications cited constitute the documentation of version 1.7 of STAT2.

*601,096*
**PB86-229960** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of Nondestructive Evaluation.
**Nondestructive Evaluation.**
Final rept.,
L. Mordfin. 1985, 25p
Pub. in Materials and Processes (3rd Edition), Part B, Chapter 30, p1495-1519 1985.

Keywords: *Nondestructive tests, Evaluation, Reprints.

No abstract available.

*601,097*
**PB87-113601** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**SEM-Based (Scanning Electron Microscope-Based) System for Calibration of Linewidth SRMs (Standard Reference Materials) for the IC (Integrated Circuit) Industry.**
Final rept.,
D. Nyyssonen, and M. T. Postek. 1985, 7p
Pub. in SPIE 565, p180-186 1985.

Keywords: *Linewidth, Electron microscopes, Calibrating, Integrated circuits, Reprints, Standard reference materials, Scanning electron microscopy.

The National Bureau of Standards is currently developing a new scanning electron microscope-based linewidth measurement system for future calibration of standard reference materials for the IC industry. This system incorporates a piezo/interferometric stage for precise translational motion and the monitoring of distance, improved vibration-isolation, microprocessor stage control system, and computer data analysis. The specifications incorporated into the system are designed for the measurement of linewidth dimensions from 0.1 to 2 um with a precision of 0.002 um. The design philosophy of the system is discussed along with the current limitations of accurate edge detection in SEM-based systems.

*601,098*
**PB87-118758** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Laser Simulation of Buried AE (Acoustic Emission) Sources.**
Final rept.,
D. A. Hutchins, K. Lundgren, R. P. Young, and N. N. Hsu. 1986, 5p
Pub. in Jnl. of Acoustic Emission 5, n3 pS29-S33 Jul/Sep 86.

Keywords: Greens function, Light pulses, Simulation, Reprints, *Acoustic emissions, Acoustooptics, Buried objects, Laser radiation.

A pulsed laser has been used to simulate AE sources both buried within metallic plates and at various solid surfaces. Waveforms detected by either interferometric or piezoelectric sensors are then discussed in terms of AE detection and source location. A comparison to wave propagation theory is also presented for the buried sources, yielding good agreement.

## Robotics/Robots

*601,099*
**PB86-195534** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
**Servoed World Models as Interfaces between Robot Control Systems and Sensory Data.**
Final rept.,
E. W. Kent, and J. S. Albus. 1984, 9p
Pub. in Robotica 2, pt1 p17-25 1984.

Keywords: *Robots, Control equipment, Feedback, Detectors, Reprints, World models.

A hierarchical robot sensory system being developed for industrial robotics is described. At each level of the hierarchy, sensory interpretative processes are guided by expectancy-generating modeling processes. The modeling processes are driven by a priori knowledge (object prototypes), by knowledge of the robot's movements (feedforward from the control system), and by feedback from the interpretative processes (prior state of the sensory world). At the lowest level, the senses (vision, proximity, tactile, force, joint angle, etc.) are handled separately; above the level, they are integrated into a multi-modal world model. At successively higher levels, the interpretative and modeling processes describe the world with successively higher order constructs, and over successively longer time periods. Each level of the corresponding levels of a hierarchical robot control system.

*601,100*
**PB86-202009** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Robot Control System Based on FORTH.**
Final rept.,
J. L. Michaloski, and B. A. Warsaw. May 86, 5p
Pub. in Robotics Engineering, p22-26 May 86.

Keywords: *Robots, *Real time operations, Computer programming, Control equipment, Reprints, Computer applications, Computer program verification.

The benefits of developing a real-time control system (RCS) using FORTH is discussed. FORTH software development is achieved through the use of small, verifiably correct modules. The FORTH programming environment is highly interactive, completely open, and easily extensible. A real time robot control system requires much software integration, fine-tuning, hardware interfacing, and robot error handling. RCS was developed using and extending FORTH because FORTH because FORTH best handled the broad and diverse programming needs of a robot control system. With FORTH as a base system, RCS provides a robot programming environment geared to reducing software complexity, simplifying program testing, and transfering the burden of programming from the user to the computer.

*601,101*
**PB86-202041** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
**Hierarchical Control of Robot Vision by Internal Models.**
Final rept.,
E. W. Kent. 1983, 7p
Pub. in Proceedings of the Annual Control Engineering Conference, Rosemont, IL., May 24-26, 1983, p263-269.

Keywords: *Robots, *Control equipment, Visual perception, Perception, Mathematical models, *Machine vision, Computer vision.

A robot sensory system developed for industrial robotics is described. Television frames and inputs from other sensors are interpreted by a hierarchically organized group of microprocessors. The system uses knowledge of object prototypes, and of robot action, to generate visual expectancies for each frame. At each level of the hierarchy, interpretative processes are guided by expectancy-generating modeling processes. The modeling processes are driven by a priori knowledge, by knowledge of the robot's movements, and by feedback from the interpretative processes. At the lowest level, other senses (proximity, tactile, force) are handled separately; above the level, they are integrated with vision into a multi-modal world model. At successively higher levels, the interpretative and modeling processes describe the world with successively higher order constructs, and over longer time periods. All levels of the hierarchy provide output, in parallel, to guide corresponding levels of a hierarchical robot control system.

*601,102*
**PB86-202058** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
**Robot Sensing for a Hierarchical Control System.**
Final rept.,
M. Shneier, E. Kent, J. Albus, P. Mansbach, and L. Palombo. 1983, 17p
Sponsored by Robotics International, Dearborn, MI.
Pub. in Proceedings of the International Symposium on Industrial Robots and Robots 7 (13th), Chicago, IL., April 17-21, 1983, v2 p14.50-14.66.

Keywords: *Robots, *Control equipment, Manipulators, Visual perception, Perception, Detectors, *Machine vision.

An hierarchical sensory system is described that is tailored to the special needs of a robot manipulator. It uses geometric models of objects and knowledge of the robot's position to generate expectations about the environment. The expectations are matched with sensory input from a variety of sources, including visual, tactile, proximity, and force and torque sensors. In the implementation, the visual sensor makes use of structured light techniques to calculate three-dimensional properties of objects. The sensory hierarchy is such that low levels deal with less-processed information than higher levels, and are expected to perform simpler tasks. At each level, the sensor input is matched with the expectations derived from the models, and the differences are used to update the understanding of the environment. Each level in the sensory-processing hierarchy communicates information to corresponding levels in the hierarchical control system that drives the manipulator.

*601,103*
**PB86-238847** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**RCS (Robot Control Systems): The NBS (National Bureau of Standards) Real-Time Control System.**
Final rept.,
A. J. Barbera, M. L. Fitzgerald, J. S. Albus, and L. S. Haynes. 1984, 3p
Sponsored by Society of Mfg. Engineers, Dearborn, MI.
Pub. in Proceedings of Conference on Robots 8, Detroit, MI., June 4-7, 1984, Volume 2: Future Considerations, p19.1-19.3.

Keywords: *Robots, *Control equipment, Real time operations, Interactive systems.

The National Bureau of Standards, Industrial Systems Division has designed the Real-Time Control System where high level goals are decomposed through a succession of levels, each producing strings of simpler commands to the next lower level. The bottom level generates the drive signals to the robot, gripper, and other actuators. Each control level is a separate process with a limited scope of responsibility, independent of the details at other levels, thus providing a foundation for future modular, 'plug compatible' hardware and software for robotics and other real-time sensory interactive control applications.

*601,104*
**PB86-238854** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Application Example of the NBS (National Bureau of Standards) Robot Control System.**
Final rept.,
L. S. Haynes, A. J. Barbera, J. S. Albus, M. L. Fitzgerald, and H. G. McCain. 1984, 15p
Sponsored by Naval Material Command, Washington, DC.
Pub. in Int. Jnl. of Robotics and Computer Integrated Manufacturing 1, n1 p81-95 1984.

Keywords: *Robots, *Control equipment, Automation, Reprints, *Computer aided manufacturing.

The National Bureau of Standards, Industrial Systems Division has designed the Robot Control System where high level goals are decomposed through a succession of levels, each producing strings of simpler commands to the next lower level. The bottom level generates the drive signals to the robot, gripper, and other actuators. Each control level is a separate process with a limited scope of responsibility, independent of the details at other levels, thus providing a foundation for future modular, 'plug compatible' hardware and software for robotics and other real-time sensory interactive control applications. The paper describes the first application of the NBS Robot Control System in a realistic factory environment, fully integrated with a workstation control system, database system, safety computer, gripper control system, vision system, and network.

*601,105*
**PB86-242567** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Development of a Flexible Automated Fixturing System.**
Technical rept. Jan 84-Jun 85,
A. H. Slocum, J. Peris, and A. Donmez. 1986, 18p
Pub. in SME Technical Paper MR86-126, p1-18 1986.

Keywords: *Robots, Fixtures, Positioning devices(Machinery), Reprints, Computer applications.

A computer-controlled flexible fixturing methodology is presented and a detailed design application is described. As implemented, the fixture is a vise-type system which has one fixed and one moving jaw, with robot changeable jaw faces. The system can locate and clamp most types of prismatic parts by utilizing two servocontrolled orthogonal mechanical planes and two sets of discretely located stops. The planes are: a moving jaw which is supported by a fully constrained bearing system and actuated by a hydraulic gerolermotor-powered ballscrew; and two hydraulically actuated leveling bars. The discrete stops are four sets of hydraulically actuated stops located on each jaw.

*601,106*
**PB87-128393** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.

**Estimation of the Dynamic Parameters of a Robot Joint Drive System.**
Final rept.,
N. Dagalakis, and D. R. Myers. 1986, 5p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) International Conference on Systems, Man, and Cybernetics, Atlanta, GA., October 1986, p655-659.

Keywords: *Joint(Junctions), *Robots, Systems analysis, Dynamics, Drives, Random processes, Accelerometers, Frequency response, Estimating, Parameters, Data analysis.

A system identification technique has been developed for estimating the dynamic parameters of an industrial robot joint drive system. Band limited random excitation was injected through the power amplifier of the joint drive system being analyzed. The motion of the robot link was monitored by a pair of accelerometers. The frequency response of two portions of the joint drive system was determined for two different loads.

*601,107*
**PB87-134714** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Watchdog Safety Computer Design and Implementation.**
Final rept.,
R. Kilmer, H. McCain, M. Juberts, and S. Legowik. 1984, 21p
Pub. in Proceedings of Conference on Robots 8, Volume 2: Future Considerations, Detroit, MI., June 4-7, 1984, p13.56-13.76.

Keywords: *Machining, *Robots, *Safety engineering, *Monitors, Automatic control, Performance evaluation, Auxiliary equipment(Computers), Equipment, Industrial sector, Computer applications.

There are many different aspects of safety to consider when utilizing a robot in an industrial application. In general, however, these can be categorized into the areas of personnel safety and equipment safety. The paper addresses the later category and presents one approach of providing equipment safety through the use of an auxiliary computer to monitor operations in the workstation. Such a computer system can be used to check robot operations during programming, automatic cycling, and debugging and repair to prevent unwanted conditions from occurring. The basic concepts, design and implementation of such an auxiliary computer on a robot operating in a machining workstation are described here.

## Tribology

*601,108*
**PB86-239118** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Functional Needs, Machining Conditions, and Economics of Surface Finishing.**
Final rept.,
J. Bielle, T. Vorburger, and V. Roy. 1985, 7p
Pub. in Precision Engineering 7, n1 p31-37 1985.

Keywords: *Cutting tools, *Surface finishing, Machining, Wear, Service life, Reprints, Tribology.

The authors discuss two applications of surface finish technology to industrial problems. The first involves the deterioration of tools used to shape large numbers of parts in a turning operation. After preliminary observations, the authors concluded that the waviness of the cutting surface of the tool was impeding the flow of the chip over the tool and reducing the usable life. After a change in the tool finishing conditions, its waviness was reduced considerably and the lifetime of the tool between sharpenings increased from 8000 to 53000 parts. The second case involves the degradation of flat steel tracks for rolling needle bearings in a molding machine.

## General

*601,109*
**PB87-145272** PC **A17**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Information Resources and Services Div.
**Publications of the National Bureau of Standards, 1985 Catalog.**
Rept. for Jan-Dec 85,
R. J. Pardee. Jun 86, 394p NBS/SP-305-SUPPL-17
See also 1984 Catalog, PB85-245678. Also available from Supt. of Docs as SN003-003-02737-5. Library of Congress catalog card no. 48-47112.

Keywords: *Catalogs(Publications), *Bibliographies, Aeronautics, Astronomy, Astrophysics, Atmospherics, Electronics, Electrical engineering, Physics, Mechanical engineering, *National Bureau of Standards, US NBS.

The 17th Supplement to Special Publication 305 contains full bibliographic citations including keywords and abstracts for National Bureau of Standards (NBS) 1985 papers published and entered into the National Technical Information Service (NTIS) collection. (Also included are NBS papers published prior to 1985 but not reported in previous supplements of this annual catalog.) Four indexes are included to allow the user to identify NBS papers by personal author, keywords, title, and NTIS order/report number.

# MATERIALS SCIENCES

## Adhesives & Sealants

*601,110*
**PB87-122263** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Developing Failure Criteria for the Polymers Used in Structural Adhesives.**
Final rept.,
D. L. Hunston, J. L. Rushford, S. S. Wang, and A. J. Kinloch. 1982, 5p
Pub. in Annual Conference of Reinforced Plastics/Composites Institute, the Society of the Plastics Industry, Inc. (37th), January 11-15, 1982, p1-5.

Keywords: *Adhesives, Polymers, Stress analysis, Epoxy compounds, Viscoelasticity, Reprints.

The desire to use adhesives and composites in structural applications has led to a need for a failure prediction capability for the polymers used in such systems. The initial phase of this study considered rising load experiments at different cross-head speeds and temperatures for neat and adhesive bond specimens. The results demonstrate that the data can be fit to empirical models that provide estimates of mode-1 fracture behavior. Current studies are now examining more complex loading histories and composite specimens.

## Ceramics, Refractories, & Glass

*601,111*
**PATENT-4 606 902** Not available NTIS
Department of Commerce, Washington, DC.
**Process for Preparing Refractory Borides and Carbides.**
Patent,
J. J. Ritter. Filed 3 Oct 85, patented 19 Aug 86, 5p PB86-241288, PAT-APPL-6-783 503
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Refractory materials, *Synthesis(Chemistry), *Borides, *Carbides, *Patents, PAT-CL-423-345.

Refractory borides or carbides are prepared by contacting an alkali-metal reducible metal chloride or silicon tetrachloride with boron trichloride or carbon tetrachloride in an inert solvent in the presence of an alkali metal, the metal chloride or silicon tetrachloride and the boron trichloride or carbon tetrachloride being present in an amount about stoichiometrically equivalent to the boride or carbide to be prepared and the alkali metal being present in an amount about stoichiometrically equivalent to the amount of chloride in the metal chloride or silicon tetrachloride and the boron trichloride or carbon tetrachloride, until all chloride present has reacted with the alkali metal to form alkali metal chloride.

*601,112*
**PATENT-4 606 906** Not available NTIS
Department of Commerce, Washington, DC.
**Process of Synthesizing Mixed BAO-TIO2 Based Powders for Ceramic Applications.**
Patent,
J. J. Ritter, R. S. Roth, and T. Negas. Filed 15 Nov 84, patented 19 Aug 86, 6p PB86-241270, PAT-APPL-6-671 539
Supersedes PB85-141752.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Barium titanates, *Dielectrics, *Patents, Roasting, Precipitation(Chemistry), Ferroelectric materials, Precursors, PAT-CL-423-598.

A process for producing any desired Ba/Ti mixture to be formulated as an amorphous solid which crystallizes at very low temperatures to yield a desired phase or phases is disclosed. The process yields products free of undesirable impurities and allows macroscopic production of certain phases in the baria-titania system, having exceptional high frequency dielectric properties, that were previously unattainable through solid-state high temperature production techniques.

*601,113*
**PB86-175833** PC **A07**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.
**National Prospectus on the Future of the U.S. Advanced Ceramics Industry. Proceedings of a Conference Held at Gaithersburg, Maryland on July 10-11, 1985,**
E. Ambler, L. H. Schwartz, and S. J. Schneider. Mar 86, 132p NBSIR-85/3240
Sponsored by Department of Commerce, Washington, DC. Office of Productivity, Technology and Innovation.

Keywords: *Ceramics, *Meetings, Industries, Marketing, Technology, Research and development.

Advanced ceramics are a new generation of high performance materials, widely believed to hold promise of multi-billion dollar markets. The U.S. competitive position, however, has been eroded in recent years with the prognosis for the future equally dim. To address this problem, the Department of Commerce held an industrially oriented conference, July 10-11, 1985, at which leaders in the ceramic field assessed critical competitive issues from both a technological and business viewpoint and developed approaches for improved U.S. market posture. The Conference considered electronic and structural advanced ceramic markets, with focus on cooperative mechanisms for industrial R&D. A consensus was reached on the most critical areas for research and on the necessity for inter- and intra-industrial collaboration. Assistance from DOC was requested to facilitate the implementation of cooperative research ventures. The report constitutes the Proceedings of the Conference and includes the papers presented and summary of the workshop sessions.

*601,114*
**PB86-185261** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Microstructure-Strength Properties in Ceramics: 1. Effect of Crack Size on Toughness.**
Final rept.,
R. F. Cook, B. R. Lawn, and C. J. Fairbanks. Nov 85, 12p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of the American Ceramic Society 68, n11 p604-615 Nov 85.

Keywords: *Ceramics, *Cracking(Fracturing), Mechanical properties, Aluminum oxide, Barium titanates, Glass, Microstructure, *Foreign technology.

A systematic study of the inert-strength characteristics of ceramics as a function of crack size relative to grain size has been made using controlled indentation flaws. The focus of the test program is on aluminas, with barium titanates and glass-ceramics providing support data in confirmation of general trends. On progressively diminishing the indentation load, the strengths first show a steady increase, but subsequently tend to a plateau, as the contact size begins to approach the characteristic grain size. A simple extension of conventional indentation fracture mechanics theory (incorporating residual contact stresses) is developed to describe this scale transition. The basis of the analysis is the postulated existence of a 'microstructural driving force,' grain-localized at the center of the pennylike radial crack, in direct analogy to the indentation driving force. This description provides closed-form solutions to the fracture mechanics equations, such that the data are interpretable in terms of an apparent R-curve function. Only two quantities are required to specify the function completely, one relating to the macroscopic toughness determined from large-scale crack specimens and the other to a microstructure-associated stress intensity factor. These quantities are advocated as useful reliability parameters. It is found that the second quantity can vary widely from material to material, even within a given class, to the extent that materials which show superior strength characteristics at large indentation loads may be dramatically weaker at low loads. The indications are that, at least for aluminas, the key to such weakening effects is to be found in the grain-boundary structures. The study emphasizes the need for extreme caution in extrapolating macroscopic-crack data unconditionally into the microscopic-flaw region, and for more fundamental investigations into the underlying physical processes actually responsible for the microstructural driving forces.

*601,115*
**PB86-192176** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Defects in Silicon Carbide Whiskers.**
Final rept.,
S. R. Nutt. 1984, 4p
Pub. in Jnl. of the American Ceramic Society 67, n6 p428-431 1984.

Keywords: *Silicon carbides, *Whiskers(Single crystals), Crystal defects, Twining, Reprints.

Defects in silicon carbide whiskers made from rice hulls were identified and analyzed using transmission electron microscopy. The whiskers were characterized by a high density of planar faults lying on close-packed plans perpendicular to the whisker axis. The faulting resulted in complex mixtures of beta and alpha polytypes arranged in thin lamellae normal to the whisker axis. Core regions of whiskers were often filled with small cavities ranging in size from 1-20 nm. Partial dislocations accompanied the cavities and were analyzed through specimen tilting experiments.

*601,116*
**PB86-193554** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Microstructure-Strength Properties in Ceramics: 2. Fatigue Relations.**
Final rept.,
R. F. Cook, B. R. Lawn, and C. J. Fairbanks. 1985, 8p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of the American Ceramic Society 68, n11 p616-623 Nov 85.

Keywords: *Ceramics, *Fatigue(Materials), Microstructure, Aluminum oxide, Cracking(Fracturing), Reprints.

The study of crack-size effects in aluminas and other selected ceramics in Part I is here extended to dynamic fatigue properties. Controlled flaws are used to measure the fatigue response in the large-crack (indentation-controlled) and small-crack (microstructure-controlled) regions. It is demonstrated that the 'microstructural driving forces' responsible for the R-curve behavior are readily accommodated into existing indentation fracture theories of fatigue strengths. The modified theory provides well-defined solutions for the strengths in terms of stressing rate and indentation load. Two load-invariant quantities, relating to the exponent and coefficient in an assumed power-law crack velocity function, are sufficient to define the entire data set for a given material, at all stressing rates and loads. This is demonstrated graphically by reducing such data sets onto universal fatigue diagrams.

*601,117*
**PB86-193752** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Structural Reliability of Ceramic Materials.**
Final rept.,
S. M. Wiederhorn, and E. R. Fuller. 1985, 18p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Department of Energy, Oak Ridge, TN. Advanced Research and Technology Fossil Energy Materials Program.
Pub. in Materials Science and Engineering 71, p169-186 1985.

Keywords: *Ceramics, Crack propagation, Creep rupture strength, Fracture properties, Reliability, Reprints.

The effect of materials properties on the structural reliability of ceramics is reviewed. For low temperature applications, methods for estimating reliability are in an advanced state of development. The parametric equations that are used to describe failure can be explained in terms of a crack growth model in which failure occurs primarily as the result of the growth of defects from a subcritical to a critical size.

*601,118*
**PB86-196771** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.
**Institute for Materials Science and Engineering, Ceramics: Technical Activities 1985,**
S. M. Hsu, and C. R. Hubbard. Feb 86, 81p NBSIR-85/3188

Keywords: *Ceramics, Physical properties, Performance, Chemistry, Processing, Stability.

Contents: Properties/performance, Mechanical properties; Glass and composites; Tribology; Optical properties; Structure/stability--High temperature chemistry; Structural chemistry; Ceramic powder characterization; Surface chemistry and bioprocesses; Processing--Structural science; Ceramic chemistry.

*601,119*
**PB86-202843** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Mechanical Properties Group.
**Creep and Fracture of Vitreous-Bonded Aluminum Oxide.**
Final rept.,
S. M. Wiederhorn, B. J. Hockey, R. F. Krause, and K. Jakus. 1986, 15p
Sponsored by Department of Energy, Oak Ridge, TN. Advanced Research and Technology Fossil Energy Materials Program, and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Materials Science 21, p810-824 1986.

Keywords: *Ceramics, *Aluminum oxide, Creep rupture strength, Fractures(Materials), Cracks, Creep properties, Reprints.

Creep and creep-rupture behavior of a commercial grade of glass-bonded, 96% aluminum oxide was characterized as a function of temperature and applied stress. The creep data were fitted to the classical empirical relation usually used to describe the phenomenon. None of the available theories of creep rupture provided a satisfactory description of the present set of data. Analytical electron microscopy was used to characterize the composition and structure of the material. In the as-received material the intergranular phase was a glass of nearly uniform composition. During high-temperature exposure, devitrification of the glass resulted in the formation of various crystalline phases within the intergranular region of the material. Devitrification depended on both the proximity to the surface, where it was most pronounced, and on the state of stress. From the composition of the retained glass, estimates of the viscosity of the glass at the grain boundaries were made and used, in combination with microstructural information, to compare the creep behavior with available theories of creep. The results of the paper are consistent with percolation and solution precipitation mechanisms of creep deformation.

*601,120*
**PB86-203569** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Ceramic Materials Characterization Using Small Angle Neutron Scattering Techniques.**
Final rept.,
K. A. Hardman-Rhyne, and N. F. Berk. 1986, 13p
Pub. in Proceedings of Sagamore Army Research Conference (31st), Lake Luzerne, NY., August 13-17, 1986, p257-269.

Keywords: *Ceramics, Neutron scattering, Nondestructive tests, Defects, Porosity, Densification.

The future of new high technology ceramic materials depend on understanding the structure of ceramic materials. Often ceramics have several microstructural components such as residual voids from the sintering process, inclusions or impurities from starting materials, second phases, and microcracks or cavities from temperature and/or pressure treatments. Intensive efforts in synthesizing new reproducible ceramics have resulted in fewer microstructural defects. Nevertheless the effects of temperature and pressure on these defects are not understood and can be studied with SANS facilities. The densification process can be studied in-situ for alternative procedures to eliminate defects at earlier stages of the process. These defects include the initial porosity, agglomeration and impurity effects in the compacted power which can monitor a fragile green state ceramic through the densification process in a nondestructive manner. With the use of theoretical and experimental SANS methods developed at NBS, particle and/or void sizes (0.001 to 10 microm) and volume fractions can be studied quantitatively.

*601,121*
**PB86-208519** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Ring-on-Ring Tests and the Modeling of Cladding Glass Strength by the Weibull Distribution.**
Final rept.,
E. Simiu, and D. A. Reed. 1985, 7p
Pub. in Proceedings of IUTAM Symposium on Probabilistic Methods in the Mechanics of Solids and Structures, Stockholm, Sweden, June 19-21 1984.

Keywords: *Glass, Construction materials, Strength, Loads(Forces), Fractures(Materials), Stresses, Probability distribution functions, Failure, Mathematical models.

Although ring-on-ring test results have been used in the past to obtain information on the strength of glass, no methodology has so far been developed in the literature relating explicitly such results to the load capacity of cladding glass. The main purpose of the report is to propose such a methodology. The proposed methodology makes use of recent advances in the modeling of the fracture mechanics behavior of glass and the calculation of stresses in plates exhibiting geometric nonlinearity. Two interesting findings are noted. First, owing to the way in which results of ring-on-ring tests are utilized, the relatively large varibilities typical of fracture mechanics parameters, as well as the uncertainities with respect to the shapes of surface flaws, have a minor effect on the estimation of load capacities. Second, two-parameter Weibull distributions, previously used in the literature to model the strength of glass and the load capacity of cladding panels, are not consistent with experimental results. On the other hand, three-parameter Weibull distributions model the observed glass behavior credibly.

*601,122*
**PB86-209186** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Compressive Strength and Creep Behavior of a Magnesium Chromite Refractory.**
Final rept.,
R. F. Krause. 1986, 9p
Sponsored by Department of Energy, Oak Ridge, TN. Advanced Research and Technology Fossil Energy Materials Program.
Pub. in Ceramic Engineering and Science Proceedings 7, n1-2 p220-228 1986.

Keywords: *Refractories, *Chromites, Creep properties, Strength, Strains, Compressive strength, Magnesium chromites, High temperature.

The compressive strength of a magnesium chromite refractory in nitrogen was measured by rapidly loading specimens to failure at several temperatures up to 1600C. Strength retrogression was observed at tem-

peratures above 1200C. The creep behavior of the refractory in nitrogen was measured as a function of compressive stress in the range from 1.4 to 5.6 MPa and as a function of temperature in the range from 1300 to 1600C. A nitrogen atmosphere was used to suppress distillation of CrO sub 3. Generally, the experiments were terminated when the specimens sustained from 0.01 to 0.02 creep strain. The creep strain (epsilon) at a given stress (omicron) and a given absolute temperature (T) was represented by the following function of time (t), epsilon = C traised to the m power, where (C) depends on stress and temperature. The time exponent (m) was evaluated as less than unity, indicating a strain-hardening model, and was independent of stress and temperature within the precision of measurements.

*601,123*
**PB86-209194** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Microstructural Analysis of Creep Failure in Si3N4 and SiC.**
Final rept.,
N. J. Tighe. 1984, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Army Materials and Mechanics Research Center, Watertown, MA.
Pub. in Proceedings of Annual Conference of the Microbeam Analysis Society (19th), Bethlehem, PA., July 16-20, 1984, Microbeam Analysis-1984, p127-130.

Keywords: *Ceramics, *Service life, Silicon carbides, Silicon nitrides, Fractures(Materials), Micro structure, Crack propagation, Electron microscopy, Creep properties, Failure, High temperature.

Advanced ceramics such as silicon nitride and silicon carbide are being used in high-temperature, high-stress heat-engine applications where catastophic failure must be avoided. It is necessary to develop the required design parameters and to predict lifetimes for these materials. Identification of the microstructural elements that cause failure is being carried out by analytical scanning transmission electron microscopy (STEM). Silicon carbide and silicon nitride fail by mechanisms that involve crack propagation from pre-existing flaws or from flaws that develop during the exposure to a simulated service environment. The pre-existing flaw population consists of inclusions, pores, and surface preparation damage; the flaw population that develops during exposure includes cavities, oxidation pits, microcracks, and reaction products from bonding phases and inclusions. Silicon nitride and silicon carbide are compounds of several crystalline and amorphous phases and the identification of the microstructural elements that relate to the failure mechanisms requires considerable structural and chemical analysis.

*601,124*
**PB86-214673** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Contact Fracture in Brittle Materials.**
Final rept.,
B. R. Lawn, and S. M. Wiederhorn. 1983, 15p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Proceedings of International Symposium on Contact Mechanics and Wear of Rail/Wheel Systems, Vancouver, British Columbia, July 6-9, 1982, p133-147 1983.

Keywords: *Brittleness, Fractures(Materials), Contacting, Strength, Erosion, Surface defects, Deformation, Reprints, *Brittle materials.

The nature of contact-induced surface damage in brittle materials, and the fracture mechanics principles used to describe the damage, are surveyed. The importance of understanding the elastic and plastic deformation processes which precede fracture is emphasized. Strength and erosive wear properties are intimately connected to the contact damage mechanics.

*601,125*
**PB86-230950** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Dry-Coupled Ultrasonic Elasticity Measurements of Sintered Ceramics and Their Green States.**
Final rept.,
M. P. Jones, G. V. Blessing, and C. R. Robbins. 1986, 4p
Pub. in Materials Evaluation, n44 p859-862 Jun 86.

Keywords: *Ceramics, Nondestructive tests, Modulus of elasticity, Reprints.

Original techniques have been developed enabling both shear and longitudinal ultrasonic waves to be dry-coupled, using minimal pressure, into green and sintered-state ceramics via elastomers. These techniques permitted the velocity measurements to be made at megahertz frequencies, from which the elastic moduli were calculated by use of independent density measurements. Velocity differences between samples composed completely of hard agglomerates and samples composed completely of soft agglomerates were observed for the green and intermediate sintered states but were not observed for the (near) dense states.

*601,126*
**PB86-232972** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Fatigue Strength of Glass: A Controlled Flaw Study.**
Final rept.,
B. R. Lawn, D. B. Marshall, and T. P. Dabbs. 1985, 12p
Pub. in Strength of Inorganic Glass, p249-260 1985.

Keywords: *Glass, *Fatigue strength at N cycles, Defects, Indentation, Reprints, Fracture(Mechanics).

The fatigue strength properties of glass containing Vickers indentation flaws are described. The responses are found to be highly sensitive to the state of the flaws, notably to the presence or otherwise of irreversible contact stresses or of deformation-induced radial cracks. When radial cracks are present (postthreshold state) the data can be described completely in terms of conventional fracture mechanics laws. Removal of the residual stresses (by annealing) results in higher strengths and reduced fatigue susceptibility. When radial cracks are not present (subthreshold state), as is the case at sufficiently small contact loads, the data deviate from the extrapolated predictions of macroscopic crack theory. The observed strengths are higher than equivalent postthreshold levels, with increased fatigue susceptibility and greater scatter. It is concluded that the sharp-crack concept of flaws remains valid down to the threshold load for crack initiation, but that below the threshold it is the crack precursor processes which control the failure properties. Implications of these results concerning the mechanical response of optical fibers are considered.

*601,127*
**PB86-232980** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Indentation: Deformation and Fracture Processes.**
Final rept.,
B. R. Lawn. 1985, 20p
Pub. in Strength of Inorganic Glass, p67-86 1985.

Keywords: *Glass, *Indentation, Deformation, Fracturing, Cracks, Reprints.

A summary of recent developments in the study of indentation processes in glass is presented. Attention is focussed on ideally 'sharp' indenters, in which the contact deformation contains both reversible and irreversible components. The relative amounts of these two components are determined by the ratio of hardness to elastic modulus, and are directly measurable from the depth recovery of the impression. At high loading rates the plastic work rate may be sufficient to cause local surface 'melting'.

*601,128*
**PB86-232998** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Environmentally Enhanced Crack Growth in Glasses.**
Final rept.,
S. W. Freiman. 1985, 21p
Pub. in Proceedings of NATO Advanced Research Workshop entitled Strength of Glass, Algarve, Portugal, March 21-25, 1983, p197-217 1985.

Keywords: *Glass, *Crack propagation, Fracturing, Stress corrosion, Fracture(Mechanics).

The paper reviews current understanding of environmentally enhanced crack growth in glasses. The process is shown to lend itself to analysis by chemical reaction rate theory. The environmental dependence of the lower end of the crack velocity regime, Region I, is shown to fit a recent molecular model for a stress induced chemical reaction in SiO2. Crack growth in Region II is shown to be transport rate controlled, while above Region II, a recently proposed electrostatic model is shown to fit the data for soda-lime-silica glass. Effects of experimental variables such as pH and temperature on the slope and portion of crack growth curves are discussed.

*601,129*
**PB86-237823** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**High-Pressure Transformation Toughening: A Case Study on Zirconia.**
Final rept.,
S. Block, G. J. Piermarini, B. J. Hockey, B. R. Lawn, and R. G. Munro. Jun 86, 2p
Pub. in Jnl. of the American Ceramic Society 69, n6 pC-125-C-126 Jun 86.

Keywords: *Zirconium oxides, Ceramics, Sintering, Reprints, High pressure.

Transformation-toughened zirconia compacts have been produced using a pressure-induced phase of zirconia as the toughening agent. The high-pressure phase is retained metastably after compaction at 8.6 GPa and sintering at temperatures as low as 250C. High-pressure processing offers potential for new transformation-toughening phases in other ceramic materials.

*601,130*
**PB86-237831** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Pressure-Temperature Phase-Diagram of Zirconia.**
Final rept.,
S. Block, J. A. H. da Jornada, and G. J. Piermarini. 1985, 3p
Pub. in Jnl. of the American Ceramic Society 68, n9 p497-499 1985.

Keywords: *Zirconium oxides, Phase diagrams, Ceramics, Reprints.

The pressure-temperature phase diagram of zirconia (ZrO2) was determined under equilibrium conditions in a diamond anvil high pressure cell (DAC) equipped for heating, by optical microscopy and x-ray diffraction techniques. At room temperature zirconia transforms from the monoclinic (M) phase to a tetragonal (T') phase which is related to the well-known high temperature tetragonal structure (T) stable above 1170C at one atmosphere. The transition to the high pressure T' form is accompanied by a volume change of -3.5%. The transformation pressure is cycle dependent and also depends on whether pressure to induce the transformation is increasing or decreasing. At higher pressures (>16.6 GPa), the T' form transforms to the orthorhombic cotunnite (PbCl2) structure. The volume change at the transition is -6.7%. With increasing temperature the T' form transforms to the high temperature tetragonal form (T). The M-T' and T'-T phase boundaries were determined under hydrostatic conditions using single crystal samples. For increasing P and T, the M-T-T' triple point was located at T = 596 + or - 18 deg C and P=2.26 + or - 0.28 GPa, while for decreasing P and T, the triple point is at T = 535 + or - 25 deg C and P = 1.7 + or - 0.28 GPa.

*601,131*
**PB86-237849** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Effect of Chemical Composition on Sintering of Ceramics.**
Final rept.,
J. E. Blendell, and C. A. Handwerker. 1986, 23p
Pub. in Jnl. of Crystal Growth 75, p138-160 1986.

Keywords: *Ceramics, Aluminum oxide, Sintering, Chemical composition, Grain boundaries, Reprints.

Recent advances have been made in the understanding of sintering of ceramics. The primary advances have been in the modelling of grain boundary and surface properties and in the measurement of the effect of low levels of impurities and dopants on the energies and properties of interfaces. These results indicate that sintering is strongly affected by crystalline anisotropy, multiple transport mechanisms, complex geometries and impurity effects. In particular the effect of variable concentrations of impurities at the trace level have been found to mask the effects of changing most other systems parameters in ceramics with low intrin-

sic concentrations of defects. Experiments are described which can be used to isolate specific parameters or processes involved in sintering, such as the surface-grain boundary dihedral angle. Specific examples of impurity effects in MgO and alpha-Al2O3 are presented.

*601,132*

**PB86-238425** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Subcritical Crack Growth in Ceramics.**
Final rept.,
S. M. Wiederhorn. 1986, 7p
Pub. in Encyclopedia of Materials Science and Engineering, v6 p4714-4720 1986.

Keywords: *Ceramics, *Crack propagation, Fractures(Materials), Reprints.

The fracture of ceramic materials is often preceeded by subcritical crack growth that originates from flaws or cracks contained in the surfaces of these materials. Subcritical crack growth is usually the result of a stressed enhanced reaction between the ceramic and water in the air, and has been observed in a wide variety of ceramic materials: glasses, porcelains, oxides, silicate minerals and titanates. Because subcritical crack growth preceeds catastrophic fracture, the strength of ceramic materials is often found to be time dependent: delayed failure is observed when ceramics are subjected to a load, and strength of ceramics is observed to depend on loading rate. The effect of subcritical crack growth on the strength of ceramics can be understood by using the science of fracture mechanics, which provides methods for quantifying crack growth. Fracture mechanics also provides a logical framework for predicting the lifetime of structural ceramics that are subjected to either static or dynamic loads.

*601,133*

**PB86-240470** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Surfaces and Interfaces: Effects on Mechanical Properties of Ceramics and Glasses.**
Final rept.,
S. M. Wiederhorn. 1986, 4p
Pub. in Encyclopedia of Materials Science and Engineering, v6 p4817-4820 1986.

Keywords: *Ceramics, *Glass, Interfaces, Surface properties, Microstructure, Fracture properties, Creep properties, Reprints.

The mechanical behavior of ceramic materials at both low and elevated temperatures is influenced by the presence of surfaces and interfaces. At low temperatures where ceramics are brittle, mechanical perfection of surfaces determines the strength of ceramic materials. At elevated temperatures, where atoms move and react freely, factors such as creep and surface reactivity play a role in determining mechanical behavior. In the article, low temperature mechanical behavior of ceramic materials is discussed in terms of the microstructure of surfaces and the effect of machining, polishing and processing on the microstructure. High temperature mechanical behavior is discussed in terms of surface reactivity and grain boundary mobility and the importance of these processes to fracture, creep, and creep fracture.

*601,134*

**PB86-241718** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Fracture Toughness Testing of Brittle Materials.**
Final rept.,
S. W. Freiman. 1986, 4p
Pub. in Encyclopedia of Materials Science and Engineering, v3 p1868-1871 1986.

Keywords: *Brittleness, Toughness, Fracture properties, Tests, Reprints, Fracture toughness.

No abstract available.

*601,135*

**PB87-104915** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Problems with Cryogenic Operation of Piezoelectric Bending Elements.**
Final rept.,
C. L. Duffield, J. Moreland, and F. R. Fickett. May 86, 3p
Pub. in Review of Science Instruments 57, n5 p990-992 May 86.

Keywords: Ceramics, Cryogenics, Bending, Reprints, *Lead titanate zirconates, Bimorphs, Micropositioners.

Piezoelectric bimorphs constructed from lead titanate-zirconate (PZT) ceramic bonded to a brass sheet have been tested at cryogenic temperatures to determine their suitability for use in a low-temperature micropositioner. Experimental data are presented on bimorph sensitivity (displacement per volt) as a function of the number of temperature cycles. Results indicate that bimorphs of this type cannot be calibrated because of irreversible changes in the bending characteristics that occur while cycling from room temperature to 4 K.

*601,136*

**PB87-105029** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Characterization of Microcracks in Yttrium Chromate (III) Using Small-Angle Neutron Scattering and Elasticity Measurements.**
Final rept.,
E. D. Case, and C. J. Glinka. 1984, 7p
Pub. in Jnl. of Materials Science 19, n9 p2962-2968 1984.

Keywords: *Ceramics, *Cracks, Neutron scattering, Elastic properties, Polycrystals, Reprints, *Yttrium chromates.

The mean crack radius, crack opening displacement, number density, and volume fraction have been estimated for a population of microcracks in polycrystalline YCrO3 using small angle neutron scattering in tandem with elasticity measurements.

*601,137*

**PB87-106050** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Complex Permittivity of Beryllium-Oxide between 100-K and 300-K at 9.3 GHZ.**
Final rept.,
W. C. Daywitt. 1985, 2p
Pub. in Institute of Electrical and Electronics Engineers Transactions on Instrumentation and Measurement 34, n1 p98-99 1985.

Keywords: *Beryllium oxides, Ceramics, Dielectric properties, Reprints.

9.3 gigahertz measurement results of the relative dielectric constant and loss tangent of ceramic beryllium oxide at 99, 145, 223, and 300 kelvins are reported.

*601,138*

**PB87-118535** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Monocrystal Elastic Constants of NbC.**
Final rept.,
H. M. Ledbetter, S. Chevacharoenkul, and R. F. Davis. 1986, 4p
Pub. in Jnl. of Applied Physics 60, n5 p1614-1617, 1 Sep 86.

Keywords: *Niobium carbides, Elastic properties, Reprints.

Using ultrasonic methods at ambient temperatures, for niobium carbide the authors determined the monocrystalline elastic stiffnesses: C sub 11, C sub 12 and C sub 44 in Voigt's contracted notation. From these, the authors calculated the quasi-isotropic (polycrystalline) elastic constants and the elastic Debye characteristic temperature. Results derived from a blackman diagram suggest that ionic forces contribute significantly to the elastic constants and to interatomic bonding. This conclusion applies not only to NbC but also to other MX carbides with an NaCl-type crystal structure.

*601,139*

**PB87-118931** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Electrical Resistivity and Microwave Transmission of Hexagonal Boron-Nitride.**
Final rept.,
H. Frederikse, A. Kahn, A. Dragoo, and W. Hosler. 1985, 5p
Sponsored by Defense Nuclear Agency, Washington, DC.
Pub. in Jnl. of the American Ceramic Society 68, n3 p131-135 1985.

Keywords: *Boron nitrides, Electrical resistivity, Semiconductors, High temperature research, Energy gap, Wave propagation, Microwaves, Reprints.

The dc conductivity of hexagonal boron-nitride (BN) and BN-containing composites was measured as a function of temperature up to 2400 deg C. The results confirm that at high temperatures BN is an intrinsic semiconductor with an energy gap of 6.2 plus or minus 0.4 eV at T = 0 K. Extrapolated values for the resistivity of BN in the range 2600 to 3000 deg C are used to analyze the absorption, reflectivity, and transmissivity of a BN window when subjected to microwave radiation under atmospheric reentry conditions. It appears that the transmissivity is of the order of 1 to 10 percent at these temperatures due mainly to the high conductivity in a very thin, very hot surface layer. The transmissivity can be improved by using a composite made of boron-nitride and silica.

*601,140*

**PB87-118949** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Environmentally Enhanced Crack-Growth in Soda-Lime Glass.**
Final rept.,
S. W. Freiman, G. S. White, and E. R. Fuller. 1985, 5p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of the American Ceramic Society 68, n3 p108-112 1985.

Keywords: *Glass, Crack propagation, Reprints.

Crack-growth data is presented for soda-lime glass in various chemical environments. It is shown that the same environments which govern crack-growth rates in vitreous silica also do so in soda-lime glass. Modifier ions are shown to affect slopes and positions of the soda-lime crack-growth curves, either through changes in the properties of the Si-O bond or through changes in the elastic properties of the bridging network. Sodium ion exchange and silica dissolution are also shown to be important, particularly at low crack velocities.

*601,141*

**PB87-119749** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Comparison of the Liquid-Nitrogen Strength and the High-Stressing-Rate Strength of Soda-Lime Glass.**
Final rept.,
D. H. Roach. 1986, 2p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of American Ceramic Society 69, n8 pC-168-C-169 1986.

Keywords: *Alkali glass, *Fatigue(Materials), Ceramics, Crack propagation, Fracture strength, Reprints, *Liquid nitrogen strength, Soda lime glass.

Indentation strength testing is used to compare two methods of avoiding slow crack growth: a high-stressing-rate test under ambient conditions vs testing under liquid nitrogen. The liquid-nitrogen strength of soda-lime glass is found to be 9% greater than the high-stressing-rate strength. This is consistent with previous measurements of an increase in K(sub c) of 9.3% at liquid-nitrogen temperature. The implication of this finding regarding time-to-failure calculations is discussed.

*601,142*

**PB87-122651** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

**Predictive Phase Equilibrium Model for Multicomponent Oxide Mixtures, Part 2. Oxides of Sodium, Potassium, Calcium, Magnesium, Aluminum, and Silicon.**
Final rept.,
J. W. Hastie, and D. W. Bonnell. 1985, 32p
Pub. in High Temperature Science 19, n3 p275-306 1985.

Keywords: *Ceramics, Thermodynamics, Sodium oxides, Potassium oxides, Calcium oxides, Magnesium oxides, Aluminum oxides, Silicon oxides, Mathematical models, Reprints, *Phase equilibrium.

A new modeling approach, described in Part I of this series, for thermodynamic predictions of multicomponent, multiphase high temperature ceramic systems has been extended to include the binary to sexternary oxide mixtures of Na, K, Ca, Mg, Al, and Si. The model, which attributes negative deviations from ideal solution behavior to the formation of complex liquids and solids, is demonstrated for systems important in high temperature materials and energy technology, including coal slags, glasses, and minerals. Good agreement between the model predictions and experimental vapor pressure data is found. Predictions and comparisons with experiment concerning melting and phase composition are also given.

*601,143*
**PB87-135208** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Local Atomic Structure in Transition Metal/Metalloid Glasses: Ni-P.**
Final rept.,
L. H. Bennett, G. G. Long, M. Kuriyama, and A. I. Goldman. 1986, 25p
Pub. in Structure and Bonding in Noncrystalline Solids, p385-409 1986.

Keywords: *Glass, *Atomic structure, Chemical bonds, Density(Mass/volume), Nuclear magnetic resonance, Reprints, *Amorphous metals, *Nickel phosphorus alloys, Fine structure.

Details of the local atomic structure and some aspects of the chemical bonding have been explored in alloys representative of the important class of metallic glasses formed from transition-metals and metalloids. A large number of binary Ni-P alloys were formed as glasses over a wide composition range by many different preparation processes. NMR experiments revealed that two distinct types of glasses were formed. A representative of each type of glass was examined by EXAFS, revealing differences in structure and bonding.

*601,144*
**PB87-136628** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Static Fatigue Limit at Elevated Temperature.**
Final rept.,
T. J. Chuang, R. E. Tressler, and E. J. Minford. 1986, 9p
Grant DE-A105-800R20679
Sponsored by Department of Energy, Washington, DC.
Pub. in Materials Science and Engineering 82, p187-195 1986.

Keywords: *Ceramics, *Crack(Propagation), Crack(Fracturing), Fatigue(Materials), Construction materials, Static tests, Grain boundaries, Reprints, *Static fatigue limit.

The static fatigue limit, defined as the stress level below which prolonged service life is expected, is derived first from irreversible thermodynamics and found to be sensitive to kinetics. Existing theories of crack growth based on distinct mechanisms are summarized and discussed to give various values of the predicted static fatigue limit. Data for the static fatigue limit measured from alpha-SiC bend bar specimens tested at 1200 C are compared with those theoretical predictions. The results suggest that, for structural ceramics crept at elevated temperatures, diffusive crack growth along the grain boundary dominates the static fatigue process and provides the fundamental level for the static fatigue limit.

*601,145*
**PB87-136636** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Real-Time Ultrasonic Nondestructive Evaluation of Green State Ceramic Powders during Compaction.**
Final rept.,
M. P. Jones, and G. V. Blessing. 1986, 14p
Pub. in Nondestructive Testing Communications 2, p155-168 1986.

Keywords: *Nondestructive tests, *Ceramics, Compacting, Ultrasonic tests, Reprints.

A real-time ultrasonic technique for the nondestructive evaluation of ceramic powders during compaction has been demonstrated. Initial results indicate that this technique can detect the presence of hard agglomerates in a spray-dried alumina powder. The proposed sensor could be employed by industry to spot flawed parts prior to removing them from the die, and to provide on-line criteria for control of compaction parameters.

## Coatings, Colorants, & Finishes

*601,146*
**PB86-160983** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Quantitative Evaluation of Blistering and Corrosion in Organic Coating Systems.**
Final rept.,
M. E. McKnight, and J. W. Martin. 1984, 8p
Sponsored by Federal Highway Administration, Washington, DC.
Pub. in Proceedings of the Symposium on New Concepts for Coating Protection of Steel Structures, Lake Buena Vista, FL., January 26, 1983, American Society for Testing and Materials Special Technical Publication 841, p13-20, 1985.

Keywords: *Organic coatings, *Corrosion, Blistering, Degradation, Evaluation, Nondestructive testing, *Infrared thermography.

A nondestructive procedure using infrared thermography for detecting air and water filled blisters and localized corrosion at the coating/substrate interface is described. Deteriorated areas are observed in real time as varying gray levels on the cathode ray tube of an infrared thermographic camera or after digitization of the signal on a TV monitor. Digitization of the analog signal permits (1) image enhancement through signal averaging techniques, (2) association of gray levels with degraded areas, (3) quantitative analysis of the panel for amount, location, and type of degradation, (4) computerized storage of the digitized signal for dynamic analysis of the degraded coating and (5) graphic display of thermographic images.

*601,147*
**PB86-165206** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Non-Electrical Measurement Techniques for Assessing the State of Coating Systems Deterioration,**
M. E. McKnight, T. Nguyen, and J. W. Martin. Feb 86, 33p NBSIR-85/3293
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Degradation, *Coatings, Protective coatings, Tests.

Nonelectrical methods used to characterize early degradation in coating systems were reviewed and critiqued with respect to their ability to provide predictive in-service performance data. The methods reviewed were classified into those that measure chemical changes, coating/substrate interfacial changes, and adhesion and mechanical properties. Although many methods are used to characterize coating system degradation, very limited research has been done to relate early property changes to in-service performance. It was concluded that because of the complexity of the degradation of coating systems, a combination of methods will be needed to characterize early degradation to the extent that service-life prediction of coating systems can be based on these measurements.

*601,148*
**PB86-186772** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Prediction of the Service Life of Coatings on Steel, Part 1: Procedure for Quantitative-Evaluation of Coating Defects.**
Final rept.,
J. W. Martin, and M. E. McKnight. 1985, 8p
See also PB86-186780.
Pub. in Jnl. of Coatings Technology 57, n724 p31-38 1985.

Keywords: *Coatings, Evaluation, Degradation, Steels, Defects, Service life, Organic coatings, Reprints.

A new procedure, based on spatial statistical techniques, is proposed and demonstrated for quantitatively evaluating the degradation state of steel substrate panels protected by an organic coating. Representative output from this procedure is presented. This output includes changes in the number, size, area, and location of defects as function of time. The proposed procedure is fully compatible with existing visual procedures. The advantage of the proposed procedure is its increased precision. Attributes of the proposed evaluation procedure are discussed in terms of an ideal evaluation procedure. It was concluded that the proposed procedure (1) is simple to apply; (2) is systematic in its approach; (3) generates quantitative measures of the degradation state of a coated panel; and (4) outputs this raw data in a publishable format. Although not proven as yet, strong indications exist that the results of the proposed procedure should also be reproducible and repeatable. The major drawback of the current procedure is the long time needed for evaluating each panel. Alternatives to this procedure are discussed which could significantly reduce this time.

*601,149*
**PB86-186780** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
**Prediction of the Service Life of Coatings on Steel, Part 2: Quantitative Prediction of the Service Life of a Coating System.**
Final rept.,
J. W. Martin, and M. E. McKnight. 1985, 10p
See also PB86-186772. Sponsored by Federal Highway Administration, Washington, DC.
Pub. in Jnl. of Coatings Technology 57, n724 p39-48 1985.

Keywords: *Coatings, Predictions, Steels, Service life, Degradation, Organic coatings, Reprints.

The applicability of a reliability and life testing procedure is demonstrated for quantitatively predicting the service life of two different coating systems. By subjecting an acrylic and an alkyd coating system to three temperatures and 95 percent relative humidity, it is experimentally demonstrated that the proposed procedure is capable of quantitatively estimating the maximum service life, at 95 percent relative humidity over a wide range of temperatures, beyond which a specified proportion, 1-, of the nominal coating populations will survive. An important result of this research is that the form of the Weibull parameter acceleration factors is the same for both coating systems, indicating that a range of organic coating systems may be governed by the same acceleration factors. It is concluded that the extension of this procedure to include other coating systems and other degradation factors is possible.

*601,150*
**PB86-192432** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Ellipsometric Studies of Chelating Inhibitor Effects on the Cathodic Delamination of an Organic Coating on Iron.**
Final rept.,
J. J. Ritter. 1984, 6p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of Coatings Technology 56, n714 p55-60 1984.

Keywords: *Acrylic coating, Chelating inhibitors, Anodization, Reprints, *Cathodic delamination, Ellipsometry.

Qualitative ellipsometry has been used to study the effects of chelating inhibitors on the cathodic delamination of an acrylic coating from an iron surface. Chelating inhibitors, such as 8-hydroxyquinoline and 2,5 dimercapto 1,3,4 thiadiazole, when dispersed in the coating, were observed to delay the onset of delamination. A similar beneficial effect was noted with a two-

layer system employing a zinc chromate primer. However, when applied by an anodic pretreatment procedure, these chelating inhibitors were relatively ineffective. Catechol was found to be an ineffective inhibitor, whereas 4-methylcatechol exhibited impressive inhibition when applied in the two-step anodization pretreatment process.

*601,151*
**PB86-201381** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Ex-situ and In-situ Sample-and-Detector Chambers for the Study of Passive Films Using Surface EXAFS.**
Final rept.,
G. G. Long, J. Kruger, and M. Kuriyama. 1983, 5p
Pub. in Proceedings of the International Symposium on Passivity of Metals and Semiconductors (5th), Bombannes, France, May 30-June 3, 1983, p139-143.

Keywords: *X-ray spectroscopy, *Films, Metals, Surface properties.

Two sample-and-detector chambers for the study of surface films on metals using x-ray absorption spectroscopy are described. Results have been obtained using both a high intensity rotating anode x-ray generator and using the Cornell High Energy Synchrotron Source (CHESS).

*601,152*
**PB86-201761** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Plasma Arc Carbide Coatings on Titanium.**
Final rept.,
R. D. Shull, P. A. Boyer, L. K. Ives, and K. J. Bhansali. 1984, 5p
Pub. in Proceedings of the Plasma Processing and Synthesis of Materials, Boston, MA., November 15-17, 1983, v30 p297-301 1984.

Keywords: *Abrasivon resistant coatings, *Protective coating, *Titanium, *Plasma spraying, Arc spraying, Chromium carbides, Titanium carbides, Tungsten carbides, Hard surfacing, Wear.

The plasma transferred arc process (PTA) has been traditionally used to deposit wear resistant coatings on iron base alloy substrates, but has not been employed to coat light weight alloys due to processing problems. In the current study, use of the PTA process to deposit TiC, WC, and Cr3C2 coatings on titanium substrates has been explored. The resistance of these coatings to dry abrasive wear has been measured and compared to that of the base metal. The variation in wear resistance of these coatings is discussed in terms of the carbide particle size and the microstructure of the deposit. A comparison is made between the coatings prepared by the present process and coatings prepared by a laser surface melting and carbide particle injection process.

*601,153*
**PB87-118121** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Kinetics of Cure of Resins and Varnishes by Differential Scanning Calorimetry.**
Final rept.,
J. H. Flynn. 1985, 2p
Pub. in Polymer Preprints 26, n1 p6-7 1985.

Keywords: *Reaction kinetics, *Drying oils, *Varnishes, Polymerization, Curing, Coatings, Thermal analysis, Inks, Reprints, Differential scanning calorimetry, Itaglio inks.

The differential scanning calorimeter (DSC) is ideal for measuring the cure of the drying oils and varnishes in currency inks since it measures these oxidative catalyzed polymerization reactions with great sensitivity. However, the cure reaction takes place mainly at the oxygen-ink interface and deep curve depends on the permeation of oxygen through a highly crosslinked skin. These factors complicate the kinetics and make it difficult to measure to total heat and degree of cure. Special fused silica cells of constant surface area and constant depths of 5 to 80 micrometers have been constructed to circumvent these complications. Temperature jump techniques have been used for the first with the DSC. Equations are developed for direct cure fitting of rate-time data and tables are given of time ratios for determining kinetic parameters. Examples of these techniques are applied to the cure of inks and their drying oil components.

*601,154*
**PB87-128203** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Plating on Aluminum: A Review.**
Final rept.,
D. S. Lashmore. 1985, 4p
Pub. in Plating and Surface Finishing 72, n6 p36-39 1985.

Keywords: *Aluminum coatings, Electrodeposited coatings, Metal coatings, Reprints.

A review of the current technology used to electrodeposit metallic coatings on aluminum is presented. For many years the zincate process seemed to dominate the industry and this trend seems to be continuing with alloy coatings containing zinc, copper, iron, and nickel. Problems in alloy sensitivity continue with the zincate process and are even more severe in anodic processes. Even so, some alloys can be coated using a phosphoric acid anodizing process as a pretreatment to plating.

*601,155*
**PB87-134243** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Surface Reactions in Discharge and CVD Deposition of Silane.**
Final rept.,
A. Gallagher. 1986, 8p
Pub. in Mat. Res. Soc. Symp. Proc. 70, p3-10 1986.

Keywords: Surface chemistry, Polymeric films, Substrates, Silanes, Discharge, *Amorphous silicon, *Chemical vapor deposition, *Surface reactions.

Glow discharge deposition of hydrogenated amorphous silicon films involves; (A) the electron collisions which produce the reactive species, (B) the gas reactions these species undergo while diffusing or drifting to the surfaces, and (C) the surface reactions involved in film growth and gas processing. The author will first describe our knowledge of the electron and gas reactions in these discharges, then of the surface reactions, and finally the author will offer some conjectures regarding the influence of these different surface reactions and bombardments upon film properties.

## Composite Materials

*601,156*
**PB86-231545** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Polymer Composites--Challenges and Research Trends.**
Final rept.,
D. Hunston, R. Dehl, and W. L. Wu. Mar 86, 5p
Pub. in Mechanical Engineering, p52-56 Mar 86.

Keywords: *Composite materials, Polymers, Research, Measurement, Plastics processing, Reprints.

The application and growth of polymer composites are hindered by problems associated with fabrication and performance prediction capabilities. A major source of these problems is the lack of basic knowledge concerning the relationships among processing, and properties. Research at the National Bureau of Standards is helping to address the need by developing test methods and by using these methods to generate scientific data on model materials. The program involves efforts in three areas. First, processing is being studied by developing measurements to monitor cure and by simultaneously applying these tests to study model systems. Second, measurement methods for the analysis of molecular structure, morphology, and defect content in composite materials are being investigated. Finally, performance properties are being measured and characterized. These studies are used to generate processing-structure-property relationships that will facilitate more rapid and reliable fabrication of composites.

*601,157*
**PB86-238409** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Effective Wave Speeds in an SiC-Particle-Reinforced Al Composite.**
Final rept.,
H. M. Ledbetter, and S. K. Datta. 1986, 10p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Jnl. of Acoustical Society of America 79, n2 p239-248 Feb 86.

Keywords: *Particulate composites, Composite materials, Wave propagation, Plane waves, Elastic properties, Reprints, Aluminum matrix composites, Silicon carbide reinforced composites.

Plane-wave propagation in an SiC-particle-reinforced aluminum-alloy composite was studied. Considering the composite to possess orthotropic symmetry (nine independent elastic constants), by a pulse-echo method, nine independent ultrasonic velocities were measured. Measured elastic stiffnesses departed negatively up to 40% from a rule-of-mixture model. Using ensemble-average, scattered-plane-waves methods, the composite was modeled as SiC particles represented as prolate spheroids distributed randomly, both in position and in orientation. Wave speeds of plane waves, both longitudinal and shear, were calculated in the long-wavelength limit. These wave speeds lead to equations for the effective static bulk and shear moduli of the composite. Further, a nonhomogeneous particle distribution was considered. Wave-speed equations were derived for the case where the composite contains particle-free aluminum-alloy regions that were represented by oblate spheroids.

*601,158*
**PB86-238417** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Internal Strain (Stress) in an SiC/Al Particle-Reinforced Composite.**
Final rept.,
H. M. Ledbetter, and M. W. Austin. 1986, 8p
Pub. in Advances in X-ray Analysis, v29 p71-78 1986.

Keywords: *Residual stress, *Particulate composites, Composite materials, Strains, Reprints, Aluminum matrix composites, Silicon carbide reinforced composites.

Silicon carbide and 6061 aluminum alloy possess very different thermal-expansion coefficients: 3.3 and 22.5x0.000001/K, respectively. Thus, one expects large internal strains and stresses in these composites because the two constituents form interfacial bonds at high temperatures and are cooled to ambient temperatures. From a simple elastic model, one expects a hydrostatic tensile stress in the aluminum matrix and a hydrostatic compressive stress in the silicon-carbide particles. Using conventional diffraction geometry, using Cu kalpha radiation, the authors studied three surfaces of a plate specimen. For both phases, the authors determined the unit-cell dimensions for two situations: unmixed and mixed in the final composite.

*601,159*
**PB87-111662** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Elastic Constants and Internal Friction of Reinforced Composites.**
Final rept.,
H. M. Ledbetter. 1985, 6p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Jnl. de Physique 46, n12 pC10-573-C10-578 Dec 85.

Keywords: *Composite materials, Internal friction, Elastic properties, Fiber composites, Reprints.

The authors describe experimental studies on the anisotropic elastic constants and internal friction of reinforced composites. Reinforcement types include fiber and fabric. Studied materials include boron-aluminum, glass-epoxy, boron-epoxy, graphite-epoxy, and aramid-epoxy. The authors made most measurements with a Marx three-component oscillator at kilohertz frequencies. In all cases, elastic-constant direction dependence fit relationships derived for homogeneous monocrystals. Usually, elastic stiffness and internal friction show an inverse relationship. In no case did the inclusion-matrix interface appear to contribute significantly to internal friction.

*601,160*
**PB87-111670** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Young Modulus and Internal Friction of a Fiber-Reinforced Composite.**
Final rept.,
H. M. Ledbetter, M. Lei, and M. W. Austin. 1986, 5p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Jnl. of Applied Physics 59, n6 p1972-1976, 15 Mar 86.

Keywords: *Fiber composites, Modulus of elasticity, Internal friction, Fiberglass reinforced plastics, Reprints, Epoxy matrix composites.

By a kilohertz-frequency resonance method the authors determined the Young modulus and internal friction of a uniaxially fiber-reinforced composite. The composite comprised glass fibers in an epoxy-resin matrix. The authors studied three fiber contents: 0, 41, and 49 vol %. The Young modulus fit a linear rule of mixture. The internal friction fit a classical free-damped-oscillator model where one assumes a linear rule of mixture for three quantities: mass; force constant; and mechanical-resistance constant.

*601,161*
**PB87-112314** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Fire Characteristics of Composite Materials - A Review of the Literature,**
J. E. Brown, J. J. Loftus, and R. A. Dipert. Aug 86, 46p NBSIR-85/3226
Sponsored by Naval Sea Systems Command, Washington, DC.

Keywords: *Composite materials, *Shipboard fire control, Navy, Thermoplastic resins, Thermoset resins, Fires, Tests, Flammability.

A review is presented of the open literature concerning fire tests of composite materials which may be considered for use in U.S. Navy shipboard structures and installations. Results obtained for thermoplastic resins, thermoset resins, and composite structures are summarized from standard test methods. The methods include tests for limiting oxygen index, smoke production, flame spread, fire endurance, and also from measurements of polymer properties, including differential scanning calorimetry and thermogravimetric analysis. Typical criteria used by various investigators for ranking materials are discussed, and the material rankings based on test results are given. Data from non-standard tests designed to measure fire performance are also discussed. A detailed review of data and results of tests for selected references is given. Finally, recommendations are made for test developments and for the future direction of the U.S. Navy's fire evaluation program for composites and related materials intended for shipboard use.

*601,162*
**PB87-118618** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Composite Interlaminar Fracture: Effect of Matrix Fracture Energy.**
Final rept.,
D. L. Hunston. 1984, 5p
Contract NASA-L-31134B
Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center.
Pub. in Composites Technology Review 6, n4 p176-180 1984.

Keywords: *Fracture(Materials), *Composite materials, Crack propagation, Adhesion, Thermoplastic resins, Delaminating, Reprints, Interlaminar fracture.

The data analyzed in the paper show a definite correlation between resin mode-I fracture energy and composite interlaminar fracture energy as measured by the double cantilever beam specimen. With brittle polymers, the resin toughness is fully transferred to the composite while with tougher polymers the resin toughness is only partially transferred presumably because the fibers restrict the crack tip deformation zone in the polymer. Not surprisingly, resin toughness is not the only factor that is important in interlaminar fracture. Factors that tend to increase the interlaminar toughness are fiber nesting and bridging and fiber breakage and pull-out during crack growth. Factors that tend to lower the interlaminar fracture energy are resin porosity and weak fiber-matrix bonding.

*601,163*
**PB87-122495** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Fracture Toughness of a Steel Matrix, Titanium Carbide Composite.**
Final rept.,
R. J. Fields, D. E. Harne, and B. A. Fields. 1985, 11p
Pub. in Proceedings of Meeting of the Mechanical Failures Prevention Group, Failure Mechanisms in High Performance Materials (39th), Gaithersburg, MD., May 1-3, 1984, p117-127 1985.

Keywords: *Fracture toughness, *Titanium carbides, *Composite materials, *Steels, Matrix materials, Fracture tests.

Steel matrix-TiC composites are used in the cutwater of prototype coal slurry pumps and valves. In this application, these materials must resist erosion and fracture. While they have proved to be adequately resistant to erosion, there have been some fractures in this application. The authors have measured the fracture toughness of a 45 v/o TiC in steel metal matrix composite according to ASTM standard test method E-399. Difficulties encountered in performing these tests will be discussed. The results of using a simple hardness indentation technique to determine K(sub IC) will be compared with the E-399 results. In addition, relevant micrographs and fractographs will be presented to indicate how crack propagation occurs in this composite.

*601,164*
**PB87-128963** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Influence of Damage on Mechanical Performance of Woven Laminates at Low Temperatures.**
Final rept.,
R. D. Kriz, and W. J. Muster. 1986, 8p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Proceedings of International Cryogenic Material Conference (6th), Cambridge, MA., August 12-16, 1985, p137-144 1986.

Keywords: *Cracking(Fracturing), *Damage, Mechanical properties, Laminates, Low temperature tests, Woven fiber composites, Modulus of rupture tests, Stress strain diagrams, Fiber laminates, *Woven laminates, Glass epoxy laminates.

Large quantities of nonmetallic woven composites will be used in magnetic fusion energy structures at low temperatures. The authors predicted and measured the influence of crack formation on the mechanical performance of standard glass/epoxy laminates (G-10CR, G-11CR) at low temperatures. From experiments with tension loads, the authors studied the formation of damage as a collection of fiber breaks, fiber bundle cracks, and delaminations between adjacent fiber bundles. The authors measured fiber bundle cracks in the laminate interior and individual fiber fracture at the laminate edges. The authors discovered that the sequence and type of damage control the discontinuities ('knees') in the load-deformation (stress-strain) diagrams. The authors found that G-11CR has two knees and three distinct moduli, whereas G-10CR has only two moduli and a single knee at a lower strain than G-11CR. Decrease in moduli measured near the knees compared well with predictions from a finite element model.

*601,165*
**PB87-131868** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
**Finite Element Analysis of Curved Composite Laminate.**
Final rept.,
J. D. Lee, and B. L. Wang. 1986, 6p
Pub. in Proceedings of International Symposium on Composite Materials and Structures, Beijing (China), June 10-13, 1986, p274-279.

Keywords: *Laminates, *Composite materials, *Finite element analysis, Tension, Stresses, Strain(Mechanics), Torsion, Three-dimensional calculations.

A general purpose three-dimensional finite element computer program has been developed for the analysis and optimal design of composite structure made of arbitrarily curved composite laminate. The applicability and validity of this program are demonstrated here by solving a few sample problems: a composite tube subjected to axial tension, radial expansion, and/or torsion.

*601,166*
**PB87-132742** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Standardizing Nonmetallic Composite Materials for Cryogenic Applications.**
Final rept.,
M. B. Kasen. 1986, 6p
Sponsored by Department of Energy, Washington, DC. Div. of Magnetic Fusion Energy.
Pub. in Proceedings of Seminar on Property Evaluation and Standardization of Cryogenic Materials, Tokyo, Japan, September 2, 1986, p1-6.

Keywords: *Composite materials, Nonmetals, Standards, Cryogenics, Fracture strengths, Torsion tests.

The current status of standards for nonmetallic composite materials at cryogenic temperatures is reviewed and future needs are assessed. It is concluded that a generic system for categorizing composite materials according to their cryogenic performance would be of value to engineers. It is also concluded that standard test methods are needed for producing both component data bases and design data bases.

*601,167*
**PB87-132759** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**High Quality Organic Matrix Composite Specimens for Research Purposes.**
Final rept.,
M. B. Kasen. 1986, 4p
Sponsored by Department of Energy, Washington, DC. Div. of Magnetic Fusion Energy.
Pub. in Jnl. of Composites Technology and Research 8, n3 p103-106 1986.

Keywords: Composite materials, Mechanical properties, Fracture properties, Shear properties, Mechanical tests, Reprints, *Organic matrix composites.

An efficient method for producing and testing organic-matrix composite specimens for research purposes is described. The production method is adaptable to in-house manufacturing and provides complete control over a large variety of material and processing variables. The rod-shaped, uniaxially reinforced or neat-resin specimens may be cut to length and tested without further machining. Conventional short-beam shear, flexural strength, and compression test methods may be used. Development of test methods for performing torsinal shear tests and for determining the fracture energy, Glc, are described. Test results at room temperature and at cryogenic temperature are presented.

*601,168*
**PB87-134755** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Continuous Damage Mechanics (CDM) Model of Damage Accumulation in Laminated Composites.**
Final rept.,
M. P. Wnuk, and R. D. Kriz. 1985, 18p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in International Jnl. of Fracture 28, p121-138 1985.

Keywords: *Fractures(Materials), *Laminates, Cracking(Fracturing), Composite materials, Crack propagation, Combination laminates, Reprints, Epoxy graphite laminates.

A modified version of the Kachanov damage accumulation law is employed to study the damage kinetics in laminated composite materials such as epoxy/graphite laminates. The primary objective of the present work is to quantify the characteristic events involved in the final stages of the failure process in composite materials following occurrence of the CDS. The process of localization and spread of damage ahead of the dominant matrix crack is viewed as a sequence of nucleation and propagation phases both of which may be described by use of the internal damage parameter. This scalar quantity reflects the ratio of the current crack (or pore) density to its saturation, or critical level.

It is shown that the Continuous Damage Mechanics (CDM) approach is useful in modeling a damage field consisting mainly of the fiber breaks generated ahead of the matrix crack and clustered around the plane of a prospective fracture, thus forming the so-called 'damage band' embedded within the stress field of the dominant crack. Description of this type of damage applies to the failure process which follows formation of the 'characteristic damage state' (CDS) observed in a number of multiphase materials.

## Corrosion & Corrosion Inhibition

*601,169*
**DE85017205** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Corrosion of Materials Used in Steam Generating Boiler Systems. Final Report.**
E. Escalante, D. Mathews, and J. Fink. Oct 84, 50p
NBSIR-84-2959
Contract AT01-79CS20528
Portions of this document are illegible in microfiche products.

Keywords: *Boilers, *Incinerators, *Refuse-Fueled Boilers, Chlorides, Coal, Materials Testing, Pitting Corrosion, Stainless Steel-304, Steam Generators, ERDA/360105, ERDA/421000.

Five alloys, SA178, SA192, SA213-T11, SA213-T22, and Type 304 Stainless Steel, were evaluated on their resistance to pitting in a coal burning boiler and in a residential refuse burning incinerator. The materials were introduced into the vicinity of the boiler tubes using a probe whose temperature was controlled and monitored to simulate conditions of the boiler tubes. After three to six months, the probes were withdrawn and the alloy specimens removed for evaluation. The data indicate that the environment of the refuse burning incinerator was considerably more aggressive than that of the coal burning boiler. Chloride was found in practically all the pits examined in the alloys from the refuse burning system, but no chloride was found in the pits examined on the materials exposed in the coal burning boiler. The data suggest that the moisture from lawn clippings increases the rate of attack which is further aggravated by large temperature fluctuations. Type 304 stainless steel was the most resistant to pitting in both environments, but the SA213-T11 and SA213-T22 were less resistant to pitting than the lower alloy SA178 and SA192 in the refuse burning incinerator. (ERA citation 10:046748)

*601,170*
**PB86-193828** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Use of Load-Pulsing Technique to Determine Stress-Corrosion Crack Velocity.**
Final rept.,
P. W. Slattery, J. Smit, and E. N. Pugh. 1984, 13p
Pub. in ASTM (American Society for Testing and Materials) Special Technical Publication 821, p399-411 1984.

Keywords: *Stress corrosion, Cracking(Fracturing), Admiralty metal, Reprints.

A load-pulsing technique has been used to determine the velocity of transgranular stress-corrosion cracks in Admiralty Metal tested in a 15N aqueous ammoniacal solution. In this technique, small load pulses are periodically superimposed onto an otherwise constant tensile load during crack propagation, producing markings on the fracture surfaces which delineate the positions of the crack front.

*601,171*
**PB86-238094** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Corrosion of Zinc.**
Final rept.,
J. Kruger. 1986, 1p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p914 1986.

Keywords: *Corrosion, *Zinc, Reprints.

No abstract available.

*601,172*
**PB86-238102** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Corrosion of Tin.**
Final rept.,
J. Kruger. 1986, 1p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p912 1986.

Keywords: *Corrosion, *Tin, Reprints.

No abstract available.

*601,173*
**PB86-238110** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Corrosion of Magnesium.**
Final rept.,
J. Kruger. 1986, 2p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p904-905 1986.

Keywords: *Corrosion, *Magnesium, Reprints.

No abstract available.

*601,174*
**PB86-238128** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Corrosion of Lead.**
Final rept.,
J. Kruger. 1986, 1p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p904 1986.

Keywords: *Corrosion, *Lead(Metal), Reprints.

No abstract available.

*601,175*
**PB86-238169** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Chemical and Electrochemical Aspects of SCC of Alpha-Brass in Aqueous Ammonia.**
Final rept.,
U. Bertocci, and E. N. Pugh. 1984, 9p
Pub. in Proceedings of International Congress on Metallic Corrosion (9th), Toronto (Canada), June 3-7, 1984, p144-152.

Keywords: *Brasses, *Stress corrosion, Ammonia, Electrochemistry.

The chemistry and electrochemistry of the brass-ammonia system have been reviewed and up-dated. It is concluded that the cupric ammonium complex whose presence is necessary for the occurrence of cracking under open-circuit conditions in conventional oxygenated solutions simply provides a cathodic reaction, permitting cracking either by the film-rupture model or by a mechanism involving dezincification. It is shown that cracking can also occur in deoxygenated solutions in the absence of significant concentration of the cupric ions provided that cuprous complexes are present, and it is suggested that the role of the cuprous complex is again to provide a cathodic reaction, in the case allowing dezincification to occur. These findings are consistent with the recognition that stress-corrosion failures of brass are not specific to ammonia.

*601,176*
**PB86-238177** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Electrochemical Principles of Corrosion.**
Final rept.,
U. Bertocci. 1986, 4p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p1403-1406 1986.

Keywords: *Corrosion, *Electrochemistry, Reprints.

No abstract available.

*601,177*
**PB86-238185** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Stress-Corrosion Cracking of Brass in Aqueous Ammonia in the Absence of Detectable Anodic-Dissolution.**
Final rept.,
U. Bertocci, F. I. Thomas, and E. N. Pugh. 1984, 2p
Pub. in Corrosion 40, n8 p439-440 1984.

Keywords: *Brasses, *Stress corrosion, Ammonia, Reprints, Copper alloy 30Zn.

Tensile tests on Cu-30Zn brass were carried out in aqueous ammonia solutions containing Cu+ ions and equilibrated with respect to copper so that no detectable dissolution of the specimens occurred. The specimens failed by transgranular stress corrosion cracking (SCC). Similar tests in deoxygenated aqueous ammonia did not show any brittle fracture. The results show that anodic dissolution of copper is not required for SCC to occur. The significance of these results in terms of various proposed mechanisms for SCC is discussed. Periodic Cu+ depletion at the crack tip is a possible cause for the experimentally observed discontinuous crack advance.

*601,178*
**PB86-238334** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Underground Corrosion.**
Final rept.,
E. Escalante. 1986, 2p
Pub. in Encyclopedia of Materials Science and Engineering, v7 p5208-5209 1986.

Keywords: *Underground corrosion, Reprints.

No abstract available.

*601,179*
**PB86-238375** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Corrosion of Metals: An Overview.**
Final rept.,
J. Kruger. 1986, 6p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p905-910 1986.

Keywords: *Corrosion, Reviews, Reprints.

No abstract available.

*601,180*
**PB86-238441** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Corrosion: Metallurgical Aspects.**
Final rept.,
E. N. Pugh. 1986, 2p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p889-890, 1986.

Keywords: *Corrosion, Reprints.

No abstract available.

*601,181*
**PB86-240751** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Stress-Corrosion Cracking.**
Final rept.,
E. N. Pugh. 1986, 2p
Pub. in Encyclopedia of Materials Science and Engineering, v6 p4669-4670 1986.

Keywords: *Stress corrosion, Reprints.

No abstract available.

*601,182*
**PB86-241726** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Economic Effects of Corrosion and Other Degradative Processes.**
Final rept.,
E. Passaglia. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p1275-1277 1986.

Keywords: *Corrosion, Degradation, Economic analysis, Reprints.

No abstract available.

*601,183*
**PB87-130522** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Anaerobic Corrosion Mechanisms.**
Final rept.,
W. P. Iverson. 1986, 10p
Pub. in Argentine-U.S.A. Workshop on Biodeterioration (Concet-NSF), p33-42 1986.

Keywords: *Corrosion, *Anaerobic bacteria, *Anaerobic processes, Iron compounds, Reduction(Chemistry), Hydrogen sulfide, Phosphine, Phosphorus, Biodeterioration, Reprints, Sulfate reducing bacteria.

Anaerobic corrosion, that is corrosion in the absence of oxygen at or near neutral pH values, has been postulated to be due to the removal of hydrogen from the surface of iron by sulfate-reducing bacteria. Evidence is presented to indicate that this type of corrosion is induced instead by a volatile, water soluble, corrosive, phosphorus-containing compound produced by these organisms in addition to hydrogen sulfide. Hydrogen sulfide produces a partially protective film on iron which has a tendency to break down. When this occurs, the phosphorus compound comes in contact with the bare iron and induces corrosion. Iron sulfide film formation may be presented by the addition of ferrous ions to the culture medium, allowing immediate contact of the corrosive phosphorus compound with the iron surface. Thus, sulfate-reducing bacteria can produce both an inhibitor and an inducer of anaerobic corrosion. The chemical formation of a similarly acting corrosive phosphorus compound by the action of hydrogen sulfide on certain phosphorus compounds is also described.

## Elastomers

*601,184*
**PB86-214657** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Small Strain Behavior of Peroxide Crosslinked Natural Rubber.**
Final rept.,
G. B. McKenna, and L. J. Zapas. 1986, 8p
Pub. in Rubber Chemistry and Technology 59, nl p130-137 Mar/Apr 86.

Keywords: *Natural rubber, *Strains, Crosslinking, Mechanical properties, Strain tests, Stress analysis, Torsion, Reprints, *Peroxide/dicumyl.

The behavior of a Natural Rubber crosslinked with 5 phr dicumyl peroxide (149 deg C, 2 hrs) has been characterized in the region of small deformations in torsion. All experiments were carried out in stress relaxation at 23 + or - 10 deg C. Torque was measured at strains as low as gamma approx. equal 0.001 and the normal force was measured at strains of gamma approx. equal 0.0046. The derivatives of the strain energy density function, partial derivative of w with respect to I(sub 1) and partial derivative of w with respect to I(sub 2), were calculated from these measurements and the values reported are resultingly for values of strains which are smaller than any reported previously. Comparison is also made with reduced stress measurements in tension and compression which were reported in a prior study.

## Fibers & Textiles

*601,185*
**PB86-240074** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Apparel Flammability: Accident Simulations and Bench-Scale Tests.**
Final rept.,
J. F. Krasny. 1986, 17p
Pub. in Textile Research Jnl. 56, n5 p287-303 May 86.

Keywords: *Clothing, *Fire resistant textiles, Flammability, Ignition, Burning rate, Flammability testing, Apparel fabrics, Reprints.

Various apparel flammability characteristics of more than 60 fabrics were explored within the framework of the Cooperative Industry Program on General Apparel Flammability sponsored by the American Textile Manufacturers Institute. Testing consisted of apparel fire simulations on a full size mannequin and a device simulating a moving leg, as well as laboratory measurements of ignition time, heat release, weight loss, and linear and area flame spread.

*601,186*
**PB87-107918** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Insulative Values of Double Layers of Fabrics Exposed to Radiative Heat.**
Final rept.,
R. M. Perkins, J. F. Krasny, and E. Braun. 1980, 9p
Pub. in Proceedings of the Annual Meeting Information Council on Flammable Fabrics (13th), Atlanta, GA., December 1979, p88-96 1980.

Keywords: *Fabrics, Apparel fabrics, Heat, Burns(Injuries), Layers.

Single and double layers of fabrics were exposed to a radiative heat flux for 2 minutes. The time to burn injury and the total heat transferred through the fabric to a heat sensor were measured.

## Iron & Iron Alloys

*601,187*
**AD-A160 831/4** PC **A04**/MF **A01**
National Bureau of Standards (IMSE), Gaithersburg, MD. Fracture and Deformation Div.
**Effect of Heat Treatment on Mechanical Properties and Microstructure of Four Different Heats of ASTM A710 Steel.**
Final rept.,
G. E. Hicho, C. H. Brady, L. C. Smith, and R. J. Fields. Sep 85, 58p Rept no. DTNSRDC/SME-CR-05-85

Keywords: *Heat treatment, *Low alloy steels, Age hardening, Electrons, Metallography, Fracture(Mechanics), Heat, Steel, Microstructure, Fine grained materials, Grain size, Mechanical properties, Fractography, Tensile properties, Test and evaluation, Thermomechanics, High strength alloys, Chemical properties.

A710 is an high strength low alloy steel whose strength is a result of both a fine grained microstructure and a dispersion of copper precipitates. For these reasons, the tensile and impact properties of an A710 plate depend as much on the thermo-mechanical history of each plate as on the chemistry of each heat. Since plates shipped from steel suppliers are frequently heat treated under different conditions, it is difficult to attribute property differences to chemistry variations rather than to heat treatment variations or vice versa. Heat to heat property differences must be determined for a specific, known heat treatment. This report describes the variability in the mechanical properties of four plates (representing four heats of steel) that have received known, and carefully controlled, heat treatments at the National Bureau of Standards. The sensitivity of these properties to heat treatment variations within each heat of steel is also reported here. Optical and electron metallographic techniques were used to determine as-received and heat treated microstructures. Scanning electron fractography was used to ascertain the fracture mechanism in the tensile and impact tests. This report also contains two appendices in which splitting fracture and microchemistry observations in A710 are discussed.

*601,188*
**PB86-189131** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Institute for Materials Science and Engineering.
**Fundamentals of Fracture.**
Final rept.,
R. Thomson, and I. H. Lin. 1985, 58p
Pub. in Hydrogen Degradation of Ferrous Alloys, p454-511 1985.

Keywords: *Fracture(Materials), Dislocations(Materials), Cracks, Reprints, Fracture(Mechanics).

The fundamentals of fracture are presented with an emphasis on atomic models and dislocation interactions with cracks. The general fundamental principles are presented with some discussion of application to the hydrogen problem.

*601,189*
**PB86-196623** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Application of Pulse-Echo Ultrasonics to Locate the Solid/Liquid Interface During Solidification and Melting of Steel and Other Metals.**
Final rept.,
R. L. Parker, J. R. Manning, and N. C. Peterson. Dec 85, 15p
Pub. in Jnl. of Applied Physics 58, n11 p4150-4164, 1 Dec 85.

Keywords: *Steels, *Ultrasonic tests, Solidification, Melting, Metallography, Interfaces, Reprints.

The velocity of sound and the density have values that are sufficiently different for liquid as compared to solid phases of metals and alloys to permit the use of pulse-echo ultrasonic techniques to locate the solid/liquid interface during solidification and melting. Experimental results are presented for pulse-echo observation of the melting and freezing of pure iron, 304 stainless steel, and tin, using Bridgman-type furnaces with unidirectional heat flow, at frequencies from 1 to 5 MHz. For both iron and steel, rapid grain growth in the solid phase at high temperatures can strongly attenuate the sound waves and can also produce backscattered waves which obscure the identification of the solid/liquid echo. Additionally, in alloys the presence of a 'mushy zone' rather than a sharp interface further reduces the reflected signal. These signal/noise problems were successfully overcome by the use of a transducer spatial scanning technique with computer signal averaging that permits the interface to be located even in concentrated alloys.

*601,190*
**PB86-196813** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**White-Beam Synchrotron Topography of Metals and Alloys.**
Final rept.,
W. J. Boettinger, H. E. Burdette, and M. Kuriyama. 1984, 11p
Pub. in Appl. X-ray Topogr. Methods Mater. Sci., p283-293 1984.

Keywords: *Topography, *Microstructure, Iron alloys, Aluminum containing alloys, Recrystallization(Metallurgy), Grain growth, Synchrotron radiation, X ray diffraction, Reprints.

Some applications of white beam synchrotron topography, performed at the Cornell High Energy Synchrotron Source (CHESS), to the microstructural characterization of metals and alloys will be described. The general quality of the x-ray topographs is shown with examples from Fe-24wt%Al samples. Topographs have also been obtained from 100 m diameter Sn powder samples. These powders were prepared by the Perepezko droplet-emulsion technique for obtaining large undercooling of liquid metal prior to solidification. Most of the powders are single crystals as determined from the topographs, but a small fraction are composed of two or three crystal grains. Multiphase alloy powders have also been examined. In situ recrystallization and subsequent grain coarsening of Al has been recorded on video tape using white beam synchrotron topography. The time evolution of the sizes of a number of crystal grains during heat treatment is determined. Simultaneous coarsening and recrystallization of a sample is seen to occur.

*601,191*
**PB86-201746** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Ostwald Ripening of Rapidly Solidified Solid-Liquid Mixtures.**
Final rept.,
P. W. Voorhees, and M. E. Glicksman. 1983, 15p
Sponsored by Metallurgical Society of AIME, Warrendale, PA., and American Society for Metals, Metals Park, OH.
Pub. in Proceedings of the Fall Meeting of the Metallurgical Society of AIME (American Institute of Mining,

Metallurgical, and Petroleum Engineers, Inc.) Chemistry and Physics of Rapidly Solidified Materials, St. Louis, MO., October 26-27, 1982, p63-77.

Keywords: *Curing, Metallurgy, Mixtures, Solidification, Curvature, Morphology, Temperature measurement, *Foreign technology, *Rapid solidification.

A new theory of Ostwald ripening in two-phase mixtures has been developed which explicity accounts for the diffusional interactions between the dispersed coarsening second phase. The theory predicts the morphology of coarsening solid/liquid mixtures in terms of time invariant distributions of interfacial curvature. The theory also predicts a dependence of the curvature distributions and ripening kinetics on the volume fraction solidified. Experiments were performed to measure the response of an ultra-precise thermal probe immersed in the coarsening rapidly solidified solid/liquid mixture over a wide range of fraction solids. Through the theory it is now possible to interpret the experimental results to gain a deeper insight into the nature of Ostwald ripening following rapid solidification.

*601,192*
**PB86-232717** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Stainless-Steel Elastic Constants at Low Temperatures: A Review.**
Final rept.,
H. M. Ledbetter. 1982, 4p
See also PB83-106070. Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Proceedings of International Cryogenic Materials Conference, Kobe, Japan, May 11-14, 1982, p112-115.

Keywords: *Stainless steels, Elastic properties, Poisson ratio, Modulus of elasticity, Reprints.

The authors review recent NBS studies on austenitic-stainless-steel elastic constants at low temperatures. By measuring velocities of longitudinal and shear waves, the authors determined accurately the usual engineering elastic constants: Young modulus, shear modulus, bulk modulus (reciprocal compressibility), and Poisson ratio.

*601,193*
**PB87-108163** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Predicting the Toughness of SMA Austenitic Stainless Steel Welds at 77 K.**
Final rept.,
T. A. Siewert. Mar 86, 6p
Pub. in Welding Jnl. 65, n3 p23-28 Mar 86.

Keywords: *Austenitic stainless steels, *Welded joints, Cryogenics, Toughness, Welding, Stainless steels, Shielded metal arc welding, Statistical analysis, Reprints.

The austenitic stainless steels often provide the best combination of strength and toughness for cryogenic applications, however, the weld toughness is frequently much lower than that of the base metal. The study proposed a more accurate and simpler model for predicting improved filler metal compositions. Several previous studies of the weld toughness have been analyzed separately and in combination using a stepwise regression method and an expanded variable list.

*601,194*
**PB87-108171** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Alternative View of Diffusion-Induced Grain Boundary Motion.**
Final rept.,
M. B. Kasen. 1986, 5p
Pub. in Philosophical Magazine A 54, n1 pL31-L35 1986.

Keywords: *Grain growth, *Grain boundaries, Diffusion, Transformations, Solutes, Motion, Migrations, Reprints, *Diffusion induced grain boundary motion.

Diffusion-induced grain boundary motion (DIGM) is interpreted as the manifestation of a solute-induced structural transformation within the boundary. The transformation results in a supersaturation of the daughter phase, which is alleviated by a reduction in excess solute by grain boundary migration. This produces the high concentration of solute observed in the wake of the boundary. A reversal of boundary motion upon reversal of the diffusion process is attributed to depletion of the boundary solute content to below the equilibrium level, causing the boundary to migrate through the high solute field to regain equilibrium. Inability to repeat the DIGM cycle is interpreted as evidence that the solute-induced transformation cannot be repeated. Evidence is provided that the solute-induced structural transformation giving rise to the DIGM process also occurs during conventional grain growth.

*601,195*
**PB87-118543** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Cryogenic Steels for Superconducting Magnets: Developments in Japan.**
Final rept.,
H. I. McHenry. 1985, 21p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in ONRFE (Office of Naval Research Liaison Office) Scientific Bulletin 10, n2 p122-142 1985.

Keywords: *Steels, Cryogenics, Superconducting magnets, Stainless steels, Reprints.

The Japan Atomic Energy Research Institute initiated a program in 1982 to develop cryogenic steels for use in the large superconducting magnets planned for the Fusion Experimental Reactor. The target properties for the cryogenic steels are a yield strength of 1200 MPA at 4 K and a fracture toughness of 200 MPa/m at 4 K.

*601,196*
**PB87-118592** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Mechanical and Swelling Behaviour of Well Characterized Polybutadiene Networks.**
Final rept.,
G. B. McKenna, and J. A. Hinkley. 1986, 9p
Pub. in Polymer 27, p1368-1376 Sep 86.

Keywords: *Polybutadiene, Synthetic elastomers, Swelling, Elastic properties, Reprints.

Endlinking of hydroxyl-terminated polybutadiene with the appropriate isocyanate has been used to prepare well characterized networks. Two networks have been studied with molecular weights of the prepolymers being 6100 and 2400 g/mole by g.p.c. Cylindrical specimens were prepared and the derivatives of the stored energy function with respect to the stretch invariants were determined by torque and normal force measurements in torsion. From these data the Valanis-Landel stored energy function derivatives w prime (lambda) were determined for both networks. The stored energy function for the junction constraint model of Flory, which is a special form of the Valanis-Landel function, has been fitted to that determined from the experiments. The contributions, Delta A sub ph and Delta A sub c to the stored energy function from the phantom network and from the junction constraints respectively do not agree with predictions from the topologies of the networks. In spite of this the form of w prime (lambda) for the junction constraint model gives an excellent 'curve fit' to the data. Comparison is also made with equilibrium swelling.

*601,197*
**PB87-119111** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Strength-Toughness Relationship for Austenitic Stainless Steel Welds at 4 K.**
Final rept.,
R. L. Tobler, T. A. Siewert, and H. I. McHenry. 1986, 4p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Cryogenics 26, p392-395 Jul 86.

Keywords: *Austenitic steels, *Welded joints, Mechanical properties, Fractures(Materials), Toughness, Cryogenics, Reprints, Low temperature.

Cryogenic mechanical property data compiled at the National Bureau of Standards, USA, have been used to analyse the relationship between yield strength and fracture toughness for austenitic stainless steel welds at 4 K. The study demonstrates that there is an inverse linear correlation between yield strength and fracture toughness for the stainless steel welds at 4 K, and that the welds have significantly lower toughness than base materials of comparable strength.

*601,198*
**PB87-119129** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Automatic Near-Threshold Fatigue Crack Growth Rate Measurements at Liquid Helium Temperature.**
Final rept.,
R. L. Tobler, and Y. W. Cheng. 1985, 7p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in International Jnl. of Fatigue 7, n4 p191-197 Oct 85.

Keywords: *Test equipment, *Crack propagation, *Austenitic steels, Fatigue(Materials), Liquid helium, Cryogenics, Reprints, Computer applications, Low temperature.

The development of a fully automated test apparatus for near-threshold fatigue crack growth rate measurements in a liquid helium environment is described, and some initial results for AISI 300 series stainless steels are presented. The experimental apparatus consists of a servohydraulic test machine and a cryostat, complete with a minicomputer, a programmable arbitrary waveform generator, a programmable digital oscilloscope and a fully automatic liquid helium refill system. The technique uses 6.4 mm thick compact specimens subjected to systematically decreasing loads, with 24 h operation at 40 Hz, the crack growth being continuously monitored by specimen compliance measurements.

*601,199*
**PB87-119152** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Low-Temperature Sound Velocities in 304-Type Stainless Steels: Effect of Interstitial C and N.**
Final rept.,
H. M. Ledbetter. 1986, 6p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Res Mechanica 18, p245-250 1986.

Keywords: *Stainless steels, *Acoustic velocity, Interstitials, Cryogenics, Reprints, Low temperature, Steel 304.

Between T = 293 and 4 K, the longitudinal ultrasonic velocity of nine 304-type stainless steels with various C-plus-N contents (0.3-1.3 atomic per cent) was measured. All alloys showed similar behavior: a regular increase in velocity down to approximately 100 K; and below this, an anomalous decrease caused by a magnetic transition. The alloys varied in two ways: (1) contrary to some reports, increasing C + N decreases the Neel temperature strongly, by approximately 13 K per atomic per cent; (2) the magnitude of the low-temperature elastic softening associated with the Neel transition decreases slightly with increasing C + N content.

*601,200*
**PB87-128948** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Fatigue Crack Initiation from Notches in Austenitic Stainless Steels.**
Final rept.,
R. L. Tobler, and Q. S. Shu. 1986, 6p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Cryogenics 26, p396-401 Jul 86.

Keywords: *Austenitic stainless steels, *Cracking(Fracturing), *Fatigue(Materials), Austentic steels, Cryogenics, Notch sensitivity, Mechanical properties, Reprints, Steel AISI 316, Steel AISI 304L.

Fatigue crack initiation from notches in austenitic stainless steels has been studied using compact specimens of two common cryogenic alloys: AISI 316 and AISI 304L. The procedure is based on a fracture mechanics technique whereby delta K rho(sub -1/2), a parameter proportional to the change in maximum elastic stress at the notch root, is correlated with the cycles to initiate a 0.254 mm crack. The effects of some experimental variables including notch radius, stress level, specimen size and test temperature (295, 76 and 4 K) are presented, and the fatigue crack initiation resistances of the AISI 316 and 304L austenitic steels are compared with martensitic and ferritic/pearlitic steel data at room temperature.

*601,201*
**PB87-134763** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Tensile and Fracture Properties of an Fe-14Mn-8Ni-1Mo-0.7C Fully Austenitic Weld Metal at 4 K.**
Final rept.,
R. L. Tobler, R. E. Trevisan, and R. P. Reed. 1985, 5p
Sponsored by Department of Energy, Washington, DC.
Pub. in Cryogenics 25, p447-451 Aug 85.

Keywords: *Austenitic steels, *Weld metals, Cryogenics, Weldments, Tensile properties, Fracture properties, Reprints, *Fracture toughness, Steel Fe 14Mn 8Ni 1Mo 0.7C.

A fully austenitic steel butt weld 21 mm thick was produced by submerged arc welding using an experimental filler metal composition: Fe-14Mn-8Ni-1Mo-0.7C. The tensile and fracture properties of the weld were measured in liquid helium to evaluate its candidacy for applications at 4 K. The yield strength (1115 MPa) and toughness (K(sub Ic) approx 192 MPa M(sub 1/2)) combination of the material compares favorably with existing base metal properties for AISI 304 type alloys. A conventional ductile fracture consisting of void formation and coalescence was shown by both tensile and fracture toughness specimens.

## Lubricants & Hydraulic Fluids

*601,202*
**PB86-241742** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Lubricants.**
Final rept.,
S. M. Hsu. 1986, 8p
Pub. in Encyclopedia of Materials Science and Engineering, v4 p2584-2591 1986.

Keywords: *Lubricants, Lubricant additives, Reprints.

Lubricants can be defined as any material which reduces friction and/or controls wear between interacting surfaces in relative motion. A lubricant functions by preventing the collision of surface asperities on opposing surfaces and can be in the form of gas, liquid or solid. There are numerous lubricants, each is specifically designed to meet certain requirements in an application. These lubricants will be described from a material standpoint.

## Materials Degradation & Fouling

*601,203*
**PB86-189156** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Wear and Related Materials Degradation.**
Final rept.,
A. W. Ruff. 1984, 53p
Pub. in Industrial Materials Science and Engineering, p299-351 1984.

Keywords: *Wear, Ceramics, Erosion, Friction, Metals, Polymers, Reprints.

A review is presented of the principal considerations concerning wear and erosion of materials. Fundamental mechanisms of wear processes in different materials are described along with theoretical developments that attempt to predict wear rates. Three different research topics in wear of materials are also summarized, involving surface modification and microstructural effects on wear.

*601,204*
**PB86-189701** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Interfacial Forces and the Fundamental Nature of Brittle Cracks.**
Final rept.,
B. R. Lawn. 1985, 3p
Pub. in Applied Physics Letters 47, n8 p809-811, 15 Oct 85.

Keywords: *Brittle fracturing, Crack propagation, Adhesion, Reprints.

A new conception of brittle fracture processes is presented. It is proposed that the crack-tip structure is immutably sharp at the atomic level, such that the attendant growth laws are uniquely determined by the stress intensity factor K of 'fracture mechanics' origin. Threshold features in the measured v(K) function for crack growth in interactive environments, previously put forward as evidence for fundamental changes in the tip structure by blunting, are shown to be more consistent with a negative K contribution from interfacial adhesive forces. These adhesive forces should be determinable from the crack velocity characteristics.

*601,205*
**PB86-201373** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Study of the Friction and Wear Behavior of Titanium under Dry Sliding Conditions.**
Final rept.,
S. R. Nutt, and A. W. Ruff. 1983, 8p
Pub. in Proceedings of the International Conference on Wear of Materials, Reston, VA., April 11-14, 1983, p426-433.

Keywords: *Titanium, *Sliding friction, *Wear, Friction, Microscopy, Deformation.

The friction and wear behavior of commercial purity titanium has been studied under dry sliding conditions. Experiments were performed using both a ball-on-flat and a block-on-ring wear test apparatus. The type of counterface material and the applied load had significant effects on the measured values of friction and wear. Scanning electron microscopy showed that titanium transferred to the counterface very early in all of the wear tests. In extended tests, this material transfer eventually generated debris which then dominated the wear behavior for the duration of the test. Transmission electron microscopy of the highly deformed region immediately beneath the worn titanium surface revealed an elongated microstructure with a strongly preferred crystallographic orientation. This deformed region was typically 1-3 micrometers thick. Extensive deformation twinning also occurred, extending up to 50 micrometers below the worn surface.

*601,206*
**PB86-237856** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Microbial Corrosion.**
Final rept.,
W. P. Iverson. 1986, 2p
Pub. in Encyclopedia of Materials Science and Engineering, v4 p3041-3042 1986.

Keywords: *Biodeterioration, Reprints.

No abstract available.

*601,207*
**PB86-238136** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Degradation, Taxonomy of.**
Final rept.,
J. Kruger. 1986, 5p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p1040-1044 1986.

Keywords: *Degradation, Taxonomy, Reprints.

No abstract available.

*601,208*
**PB86-238144** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Application of Thermal Wave Microscopy to Research on the Sliding Wear Break-In Behavior of a Tarnished Cu-15 wt% Zn Alloy.**
Final rept.,
P. J. Blau, and C. D. Olson. 1985, 7p
Pub. in Proceedings of International Conference on Wear of Materials, Vancouver, British Columbia, April 14-18, 1985, p425-431.

Keywords: *Copper zinc alloys, *Wear, Sliding friction, Microscopy, Thermal wave microscopy.

Thermal wave microscopy (TWM) is a relatively new thermal acoustic imaging technique which can be used in a specially modified scanning electron microscope (SEM) to detect subsurface features in metals and ceramics. Contrast in TWM images can be produced by differences in thermal conductivity or by subsurface defects of many kinds including pores, voids, and delaminations of layered structures. These sources of contrast makes TWM a potentially valuable tool for wear research. The current paper describes how TWM was used in conjunction with optical microscopy and SEM studies to reveal wear process differences due to sliding direction reversal in a Cu-15 wt.% Zn alloy covered by an oxide film.

*601,209*
**PB86-242583** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Wear: Modes, Behavior, and Applications.**
Final rept.,
A. W. Ruff, and K. C. Ludema. 1986, 6p
Pub. in Encyclopedia of Materials Science and Engineering, v7 p5273-5278 1986.

Keywords: *Wear, Materials, Ceramics, Reprints.

Wear is a common, costly and gradual degradative process involving loss of material and damage to which objects and machinery are generally subjected as a result of mechanical contact. While wear usually involves undesirable consequences, there are many processes of beneficial wear such as polishing, cutting and grinding. Wear, along with corrosion and obsolescence, are frequently the life-determining processes for consumer items and commercial machinery. Wear rarely involves sudden failure; hence, there is frequently acceptance of the situation that items wear out. The discussion will consider the prominent modes of wear, the different wear behavior found among different materials, and several examples of applications involving wear.

*601,210*
**PB86-242591** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Erosion.**
Final rept.,
A. W. Ruff, and G. F. Schmitt. 1986, 6p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p1573-1578 1986.

Keywords: *Erosion, Wear, Degradation, Materials, Reprints.

The term erosion or erosive wear is generally applied to material degradation through processes of solid, liquid and gas impact or flow that result in significant damage or removal of material. These processes may be either unwanted or perhaps intentionally applied as in cleaning or cutting operations. Several basic physical and chemical mechanisms have been identified in these erosion processes. It is necessary to consider the material type involved as well as the eroding media in order to establish the specific erosion mode taking place. The discussion of erosion will consider the prominent modes of erosion and the distinctions to be drawn involving different materials. It will conclude with examples of detrimental as well as beneficial erosion.

*601,211*
**PB87-134748** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Essential Work of Fracture (w sub e) Versus Energy Dissipation Rate (J sub c) In Plane Stress Ductile Fracture.**
Final rept.,
M. P. Wnuk, and D. T. Read. 1986, 11p
Sponsored by Naval Sea Systems Command, Washington, DC.
Pub. in International Jnl. of Fracture 31, p161-171 1986.

Keywords: *Fracture strength, *Cracking(Fracturing), *Crack propagation, Aluminum, Reprints.

Two measures of fracture toughness have been investigated. The first is the Cotterell's essential work of fracture (w sub e) which reflects the energy absorbed in the process of localized necking and decohesion occurring within the crack up region. The second is the familiar critical energy dissipation rate associated with the onset of crack extension and commonly designated by J. Total of 48 fracture tests have been performed on thin aluminum double-edge-notched panels and

thin compact tension specimens with varying crack size-to-ligament ratios. In a simple experimental procedure it has been established that both measures are equivalent, at least under the plane stress conditions, and that they both represent the fraction of energy which is transmitted through the plastic deformation field into the crack tip region. The ratio 'essential work of fracture/total work of fracture' has been suggested as a quantitative measure of the energy transmission process. Certain predictions are made concerning variations of the energy transmission factor during the stable phase of ductile fracture propagation.

## Miscellaneous Materials

*601,212*
**PB87-104410** PC A08/MF A01
National Bureau of Standards, Gaithersburg, MD.
**Application of a Hard Sphere Equation of State to Refrigerants and Refrigerant Mixtures.**
Final rept.,
G. Morrison, and M. McLinden. Aug 86, 159p NBS/TN-1226
Also available from Supt. of Docs as SN003-003-02753-7. Sponsored by Electric Power Research Inst., Palo Alto, CA.

Keywords: *Refrigerants, Equations of state, Computer programs, Thermodynamic properties.

The note describes the application of the Carnahan-Starling-DeSantis equation of state to halogenated hydrocarbon refrigerants and their mixtures. A complete and consistent set of thermodynamic functions is derived from the p-V-T equation of state and the perfect (ideal) gas heat capacities. A thorough discussion of reference states is included for both pure materials and their mixtures. Although this model exhibits a critical point, it does not quantitatively represent properties in the critical region. Despite this limitation, this model can represent both liquid and gaseous mixtures away from their own critical points, even at conditions near to and above the critical points of their components.

## Nonferrous Metals & Alloys

*601,213*
**DE85000592** PC A02/MF A01
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Patterns in the Occurrence of the Brittle Topologically Close-Packed Phases: Al.**
L. H. Bennett, and R. E. Watson. 1984, 12p BNL-35275, CONF-840417-9
Contract AC02-76CH00016
High-temperature alloys - theory and design conference, Bethesda, MD, USA, 8 Apr 1984.
Portions are illegible in microfiche products.

Keywords: *Heat Resisting Alloys, Aluminium Alloys, D States, Design, Embrittlement, Phase Studies, Transition Element Alloys, ERDA/360102.

Precipitation of sigma and structurally related phases can weaken or embrittle superalloys and stainless steels. These phases, known generically as topologically close-packed (TCP) structures occur in many transition-metal alloys. Methods of predicting their appearances include examination of phase diagrams and the use of d-band electron-vacancy concentrations for the transition elements. The use of an effective set of such d-vacancy values for the transition elements is reviewed. An effective d-electron vacancy value between that of Rh and Ru is assigned to the important nontransition element Al. (ERA citation 10:000871)

*601,214*
**PB86-160595** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Ignition of Metals in High Pressure Oxygen.**
Final rept.,
J. W. Bransford. 1984, 15p
Sponsored by National Aeronautics and Space Administration, Huntsville, AL. George C. Marshall Space Flight Center.
Pub. in Proceedings of National Aeronautics and Space Administration Advanced High Pressure O2/H2 Technology, Huntsville, AL., p134-148 1984.

Keywords: *Ignition, *Combustion, Liquid oxygen, Aluminum, Nickel, Stainless steels.

A description of an experimental facility used to determine the ignition and combustion characteristics of metallic materials is described. The results obtained for aluminum 6061, 302 stainless steel, and the nickel alloy-N06625-are given.

*601,215*
**PB86-189032** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Transition-Metal Alloy Formation. The Occurrence of Topologically Close-Packed Phases.**
Final rept.,
R. E. Watson, and L. H. Bennett. 1984, 13p
Pub. in Acta Metallurgica 32, n4 p477-489 1984.

Keywords: *Alloys, Transition metals, Phase, Chemical bonds, Reprints, Laves phases, Sigma phase.

The occurrence or non-occurrence of topologically close-packed (top) phases is discussed in terms of atomic volumes (V) and d-band hole counts (N sub h). The ranges of stoichiometries over which top phases occur are shown to be related to the relative sizes of the alloy constitutents. An effective N sub h is defined. It is necessary to consider the laves structures as distinct from the other top phases. The non-laves top phases have a range of favored A-to-B site volume ratios. Some suggestions are given of alloy systems in which top phases have not been reported but are expected, and vice versa.

*601,216*
**PB86-189040** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Model Predictions of Volume Contractions in Transition-Metal Alloys and Implications for Laves Phase Formation. 2.**
Final rept.,
R. E. Watson, and L. H. Bennett. 1984, 12p
Pub. in Acta Metallurgica 32, n4 p491-502 1984.

Keywords: Transition metals, Alkali metals, Alkaline earth metals, Alloys, Reprints, *Laves phases.

A simple cellular model estimate of the site volume changes attending alloying of transition metals with each other, and with alkali and alkaline earth metals is made. Application is made to AB2 (MgCu2 and MgZn2) Laves phases as well as the related AB5( CaCu5 and AuBe5) structures. Size factors and electron factors are considered as measures controlling the occurrence of Laves phases.

*601,217*
**PB86-190634** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Disorderly Crystal Structures in Transition Metal Rich-Metalloid Alloys: Implications for Glass Formation.**
Final rept.,
R. E. Watson, and L. H. Bennett. 1983, 6p
Pub. in Scripta Metallurgica 17, n7 p827-832 1983.

Keywords: *Metalloid alloys, Crystal structure, Transition metals, Reprints, Amorphous materials.

Easy glass formation usually occurs near eutectics where the glass forming temperature is close to the melting point. However, as Anderson observed(1), other factors also enter. Citing covalent systems such as SiO2 and GeS2, he noted that glass formation is favored when the crystal structure(s) of the compounds are complicated. The purpose of the present communication is to see what transition metal rich-metalloid compounds have complicated structures and what implications this might have for glass formation.

*601,218*
**PB86-192515** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Precipitation in Rapidly Solidified Al-Mn Alloys.**
Final rept.,
D. Shechtman, R. J. Schaefer, and F. S. Biancaniello. 1984, 11p
See also AD-A136 128.
Pub. in Metallurgical Transactions A: Physical Metallurgy and Materials Science 15A, n11 p1987-1997 Nov 84.

Keywords: *Aluminum alloys, Manganese containing alloys, Precipitation(Chemistry), Microstructure, Reprints, Rapid solidification.

Precipitation at 450C was studied in melt-spun ribbons containing up to 15 wt.% Mn in solid solution in Al. The as-spun ribbons were microsegregation-free at compositions up to 5 wt.% Mn, but in more concentrated alloys a cellular microstructure was present. Upon annealing, four precipitate phases are observed, some of them being found preferentially on cell boundaries and others being found within the cells. Al6MN, G and G double prime phase can coexist for long times at 450 C, but the G phase appears to be slightly more stable. A less stable T phase was detected in Al-5 wt.% Mn foils following short annealing periods. The supersaturation of the Al matrix can persist for many hours in alloys containing up to 3 wt.% Mn, but is essentially gone after 1 hour in alloys with 5 wt.% Mn or more.

*601,219*
**PB86-192960** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Diamond Anvil Cell Technology for P,T Studies of Ceramics: Zirconia (8 mol% yttria).**
Final rept.,
R. G. Munro, S. Block, G. J. Piermarini, and F. A. Mauer. 1984, 10p
Pub. in Mater. Sci. Res. 17, p783-792 1984.

Keywords: *Zirconium oxides, *Ceramics, *Aluminum oxide, Mechanical properties, X ray diffraction, Reprints.

The authors are undertaking a systematic study of the structural and bulk properties of zirconia and alumina-based materials as functions of pressure and temperature. This paper describes the experimental approach that is being taken and discusses some of the results already obtained for ZrO2 with 8 mol% Y2O3.

*601,220*
**PB86-193240** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Small-Angle Neutron Scattering Study of Phase Decomposition in the Nickel-Rich Side of the Nickel/Nickel-Aluminum (Ni3Al) Miscibility Gap.**
Final rept.,
S. P. Singhal, F. S. Biancaniello, H. A. Alperin, and H. Herman. 1985, 6p
Pub. in Scripta Metallurgica 19, n2 p133-138 1985.

Keywords: *Nickel alloys, *Aluminum containing alloys, Phase transformations, Neutrons scattering, Reprints, *Aluminum nickel, Spinodal decomposition, Temperature dependence.

Small angle neutron scattering measurements on the isothermal phase decomposition of a Ni-14.4 at %-Al alloy is in qualitative agreement with a recent nucleation theory based on cluster dynamics. The data exhibits an apparent linear temperature dependence of the power law exponents for the peak intensity and position.

*601,221*
**PB86-195005** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Phase Decomposition in Copper-Titanium Metallic Glass.**
Final rept.,
R. D. Shull, S. P. Singhal, B. Mozer, and A. Maeland. 1984, 6p
Pub. in Rapidly Solidified Metastable Mater. 28, p279-284 1984.

Keywords: *Titanium intermetallics, Phase transformations, Crystallization, Reprints, *Metallic glasses, Amorphous materials, Copper titanium.

A metallic glass ribbon of Cu55Ti45 prepared by melt spinning was examined by x-ray, neutron, and electron diffraction, by small angle neutron diffraction (SANS), transmission electron microscopy (TEM), and by differential thermal analysis (DTA). In the liquid quenched condition large angle diffraction data (both x-ray and neutron) show the broad banded structure typical of the amorphous state. The SANS data, however, exhib-

it highly anisotropic patterns arising from phase decomposition during solidification. Ribbons annealed below the glass transition temperature (T sub g) produced neutron diffraction patterns of materials with the same amorphous structure combined with a new short range order; and the SANS patterns retained the assymetry of the as-quenched material. Ribbons annealed above the crystallization temperature (T sub c) show both isotropic and anisotropic contributions to the SANS patterns. Formation of the equilibrium TiCu phase occurs directly from the metallic glass at (T sub c). The equilibrium Ti4Cu3 phase, however, forms from the TiCu phase at a just slightly higher temperature.

*601,222*
**PB86-196060** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Color Metallography of Diffusion-Induced Grain Boundary Migration in Copper-Zinc and Copper-Arsenic Alloys.**
Final rept.,
D. B. Butrymowicz, T. J. Piccone, J. R. Manning, and D. E. Newbury. 1983, 12p
Pub. in Metallography 16, n4 p349-360 1983.

Keywords: *Copper alloys, *Metallography, Arsenic containing alloys, Zinc containing alloys, Diffusion, Grain boundaries, Migrations, Reprints.

Diffusion-induced grain boundary migration is a recently recognized phenomenon which leads to unexpected motion of grain boundaries. Vastly enhanced mass transport characterizes the low temperature aspect of the phenomenon since the grain boundaries provide easy paths for diffusional redistribution of atoms in the regions traversed by the boundaries. Diffusion of a solute into or out of polycrystalline materials when only grain boundary diffusion is significant has been observed to induce grain boundaries to migrate in a number of alloys. Because the migrating boundaries sweep across grains, mixing in solute, and no compositional changes occur except in regions through which migrating boundaries pass, changes in the color of surface regions were used to detect, and to extract the extent of, the phenomenon.

*601,223*
**PB86-196821** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Mechanisms of Microsegregation-Free Solidification.**
Final rept.,
W. J. Boettinger, S. R. Coriell, and R. F. Sekerka. 1984, 10p
Pub. in Materials Science and Engineering 65, nl p27-36 Jul 84.

Keywords: *Solidification, Silver alloys, Kinetics, Reprints, Rapid solidification, Microsegregation.

Two solidification mechanisms can produce microsegregation-free crystalline alloys: planar growth and partitionless solidification. For growth at high velocity, but still with equilibrium partitioning of solute, capillarity can stabilize a planar liquid-solid interface. This type of stability, known as absolute stability, has been confirmed experimentally for Ag-Cu alloys and should apply only when the net heat flow is towards the solid. Another possibility for producing microsegregation-free alloys is partitionless solidification which can occur at high velocities and arises from the kinetics of interface motion. These kinetics involve the trapping of solute by the moving interface, causing the partition coefficient to be unity. A unified model for the variation of the interface temperature and partition coefficient with interface velocity is presented. This model spans the range from slow velocities, where local equilibrium is usually valid, to high velocities where partitionless solidification occurs. Considerations necessary to predict the conditions of microsegregation-free solidification for concentrated alloys are also discussed.

*601,224*
**PB86-197373** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Radial Distribution Studies of Amorphous Fe-W and Ni-P at High Pressure.**
Final rept.,
R. G. Munro, F. A. Mauer, G. J. Piermarini, and S. Block. 1983, 7p
Pub. in Jnl. of Applied Physics 54, n10 p5698-5704 Oct 83.

Keywords: *Distribution functions, *Iron alloys, *Nickel alloys, Load cells, X ray diffraction, Tungston containing alloys, Phosphorous containing alloys, Reprints, *Amorphous materials, High pressure.

The determination of a radial distribution function of an amorphous material contained in a diamond anvil pressure cell is discussed. The details of the method of computation are presented, and the results for two amorphous metals, Fe-W (72 at.% Fe) and Ni-P (75 at.% Ni), are presented and critically discussed. For the reduced structure function and its Fourier transform, the differential radial distribution function, amplitudes are not well determined, and maxima and minima are located with an absolute accuracy not better than three percent. However, for a single experimental configuration and sample, the relative changes in the first neighbor distance as a function of pressure are readily detectable, even for variations on the order of 0.5 percent. Measurements at 0, 0.3, 3.6, 7.5, and 10.5 GPa and room temperature indicate that Fe-W (72 at.% Fe) has a bulk modulus of about 170 GPa. Measurements at 0.15, 2.80, and 5.50 GPa indicate that Ni-P (75 at.% Ni) has a bulk modulus of about 370 GPa at room temperature.

*601,225*
**PB86-201415** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Heat Flow - Acoustic Emission - Microstructure Correlations in Rapid Surface Solidification.**
Final rept.,
R. B. Clough, H. N. G. Wadley, and R. Mehrabian. 1983, 10p
Sponsored by American Society for Metals, Metals Park, OH.
Pub. in Proceedings of the Lasers in Materials Processing Conference of the American Society for Metals, Los Angeles, CA., January 24-26, 1983, p37-46.

Keywords: *Solidification, Heat transmission, Microstructure, Acoustic emission testing, *Rapid solidification.

Heat flow models are now available for one- and two-dimensional melting and resolidification of metallic substrates subjected to high energy laser and electronbeam sources. The models can account for both stationary and moving heat sources. In the past, experimental observations have been limited to post-solidification examinations of the microstructures and have resulted in establishment of correlations between fineness of structure, interface stability and extent of altered microstructure (e.g. melt depth) with variables such as the heat flux distribution in space and time. Techniques are accordingly needed for in situ measurement of the dynamics of laser and electron beam material interactions, possibly leading to in-process control applications and the detection of defective conditions. Acoustic emission methods show promise for this. Acoustic emission accompanying absorption of 100 ms stationary electron beams of variable flux density have been measured from 1100 and 2219 aluminum alloys.

*601,226*
**PB86-201779** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Use of Metastable Phase Diagrams in Rapid Solidification.**
Final rept.,
J. H. Perepezko, and W. J. Boettinger. 1983, 18p
Pub. in Proceedings of the Alloy Phase Diagrams Symposium, Boston, MA., November 1982, p223-240 1983.

Keywords: *Solidification, Phase diagrams, Metastable state, *Rapid solidification.

During rapid solidification, the nucleation and/or growth of a thermodynamically stable phase may be difficult. In this case the liquidus, solidus or other thermodynamic data for a metastable phase are important for the interpretation and prediction of the phases present in rapidly solidified materials. In this paper various techniques are described to obtain information about metastable equilibrium from measured stable equilibrium data. Extrapolations of phase boundaries as functions of temperature, pressure or composition (including a new component) into regions of metastability can often be constructed directly on the equilibrium diagram. These constructions can be performed more quantitatively with analytical methods using thermodynamic modelling of the free energy functions consistent with measured data. A number of examples are considered including a discussion of metastable liquid miscibility gaps, metastable eutectic and peritectic reactions, pressure diagrams and metastability in ternary alloys to indicate the possible product phase selection. A coupling of metastable phase diagrams with a solidification kinetics analysis can contribute towards effective alloy design and processing during rapid solidification.

*601,227*
**PB86-208394** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Thermal Expansion of Molybdenum in the Range 1500-2800 K by a Transient Interferometric Technique.**
Final rept.,
A. P. Miiller, and A. Cezairliyan. 1985, 10p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in International Jnl. of Thermophysics 6, n6 p695-704 Nov 85.

Keywords: *Molybdenum, Thermal expansion, High temperature tests, Interferometers, Pulse heating, Reprints, Standard reference materials.

The linear thermal expansion of molybdenum has been measured in the temperature range 1500-2800 K by means of a transient (subsecond) interferometric technique. The molybdenum selected for these measurements was the Standard Reference Material SRM 781 (a high-temperature enthalpy and heat capacity standard).

*601,228*
**PB86-208436** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Relationship between Anodic Film Microhardness and Metallic Coating Adhesion on Phosphoric Acid-Anodized Aluminum Alloys.**
Final rept.,
D. E. Thomas. 1983, 4p
Sponsored by Aluminum Association, Inc., Washington, DC.
Pub. in Plating and Surface Finishing 70, n7 p53-56 1983.

Keywords: *Aluminum alloys, *Coatings, Adhesion, Anodizing, Electrodeposition, Microhardness, Reprints.

One of the most difficult problems encountered in pretreating aluminum alloys for electrodeposition using the phosphoric acid anodizing process is the determination of the process parameters for maximum coating adhesion. The paper presents a simple method for determining the approximate coating adhesion without the financial and time consuming expense of adhesion testing. Investigations show that the coating adhesion is closely linked with the anodic film microhardness. The effect of anodizing potential, anolyte temperature, anodizing time, anolyte concentration, and post anodic treatments are examined with respect to both microhardness and coating adhesion. In each case an increase or decrease in the anodic film microhardness predicts a corresponding increase or decrease in the metal coating adhesion.

*601,229*
**PB86-209293** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Chemical Principles Underlying Bioleaching of Metals from Ores and Solid Wastes, and Bioaccumulation of Metals from Solutions.**
Final rept.,
F. E. Brinckman, and G. J. Olson. 1986, 10p
Pub. in Biotechnology and Bioengineering Symposium, n16 p35-44 1986.

Keywords: *Hydrometallurgy, Metalliferous minerals, Solutions, Leaching, *Bioleaching, Biosynthesis.

A rapidly emerging though largely untapped component of biotechnology deals not only with a few light elements commonly viewed as the 'organic' part of the biosphere, but also with the remaining elements-especially the metals-that comprise the bulk of our planet and vitally influence our biosphere. Thus, current and projected research that deals with microbial interactions and processing of metals focuses on three major aspects that ties together their covalent chemistry and

molecular biotransformations: (1) metabolic utilization of metal species, (2) toxic metal resistance mechanisms, and (3) indirect metals biotransformations by exocellular metabolites. Biooxidation of lean sulfide ores and wastes by microorganisms represent powerful new cost-beneficial chemistries, as does the parallel consideration of using microorganisms to accumulate or even synthesize metal compounds in selected forms of most value to further commercial processing.

*601,230*
**PB86-209905** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Nature of Large Ti4Cu2O Particles Formed during Annealing of Cu55Ti45 Metallic Glass Ribbons.**
Final rept.,
M. J. Kaufman, and R. D. Shull. 1986, 7p
Pub. in Metallurgical Transactions A: Physical Metallurgy and Materials 17, p575-581 Apr 86.

Keywords: *Intermetallics, *Copper alloys, *Titanium containing alloys, Annealing, Crystallization, Electron diffraction, Spectroscopy, Reprints, Metallic glass.

Large particles observed in annealed Cu(sub 55)Ti(Sub 45) metallic glass ribbons have been identified using convergent beam electron diffraction and energy dispersive X-ray spectroscopy as Ti(sub 4)Cu(sub 2)O (diamond cubic, space group Fd3m), consistent with the structure derived earlier by Mueller and Knott (Trans. AIME, 1963, vol. 227, p. 674) using different experimental techniques. In addition, evidence is presented which suggests that these particles form prior to and independent of either of the two binary equilibrium phases, TiCu and Ti(sub 3) and Cu(Sub 4), which also form during the crystallization annealing treatment.

*601,231*
**PB86-209913** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Constitution of an Al-37.5Ge Splat Quenched Foil: Implications on Nucleation Kinetics.**
Final rept.,
M. J. Kaufman, M. Ellner, and H. L. Fraser. 1986, 4p
Contract DE-AC02-76ER01198
Sponsored by Department of Energy, Washington, DC. Materials Sciences Div.
Pub. in Scripta Metallurgica 20, p125-128 1986.

Keywords: *Aluminum alloys, *Germanium containing alloys, Electron microscopy, X ray diffraction, Foils(Materials), Nucleation, Kinetics, Microstructure, Solidification, Quenching(Cooling), Cooling, Reprints, Undercooling, Rapid solidification, Splat quenching.

An Al-37.5Ge splat quenched foil has been analyzed using transmission electron microscopy and X-ray diffraction. The results are supportive of previously proposed nucleation kinetics and enforce the view that the microstructures which are produced using rapid solidification can and should be related directly to the undercoolings which are achieved prior to nucleation rather than the cooling rates characteristic of the specific process. These undercoolings frequently do depend on the cooling rates of the experimental techniques and may be depicted conveniently on time-temperature-transformation diagrams.

*601,232*
**PB86-209921** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Determination of the Point Group of the Icosahedral Phase in an Al-Mn-Si Alloy Using Convergent-Beam Electron Diffraction.**
Final rept.,
L. A. Bendersky, and M. J. Kaufman. 1986, 6p
Pub. in Philosophical Magazine B: Electronic, Optical and Magnetic Properties 53, n3 pL75-L80 Mar 86.

Keywords: *Aluminum alloys, *Magnesium containing alloys, *Silicon containing alloys, Electron diffraction, Symmetry, Reprints, Point groups, Phase studies.

Convergent-beam electron diffraction has been used to determine conclusively the point group of the icosahedral phase in an Al-Mn-Si alloy. The patterns obtained clearly display the symmetries expected for the orientations of a quasicrystalline phase with the m35 point group.

*601,233*
**PB86-209939** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Analytical Electron Microscopy Study of the Recently Reported 'Ti2Al Phase' in gamma-TiAl Alloys.**
Final rept.,
M. J. Kaufman, D. G. Konitzer, R. D. Shull, and H. L. Fraser. 1986, 6p
Contract DE-AC02-76ER01198
Sponsored by Department of Energy, Washington, DC. Materials Sciences Div.
Pub. in Scripta Metallurgica 20, p103-108 1986.

Keywords: *Titanium alloys, *Aluminum containing alloys, Electron microscopy, Electron diffraction, Phase, Creep properties, Analysis, Reprints.

A variety of experimental techniques has been utilized to establish that the phase reported previously to be a new stable Ti(sub2)Al phase is instead Ti(sub2)AlN. The space group of Ti(sub2)AlN has been determined to be P6(sub3)/mmc with lattice parameters, a=0.304 nm and c=1.369 nm, in agreement with the results of Jeitschko, et al. Also, since the phase is observed only in alloys which do not contain alpha sub 2-Ti(sub3)Al, it was suggested that the solubility of N in alpha sub 2 must be rather large, while that in the gamma(TiAl) phase is low. Finally, in light of the improved creep properties of gamma alloys containing Ti(sub2)AlN precipitates, it is suggested that an increase in the volume fraction of the phase, by increasing the N and/or C contents, in these alloys might be used to enhance the mechanical properties of the normally brittle compound.

*601,234*
**PB86-229986** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Local Modes in Dilute Metal-Hydrogen Alloys.**
Final rept.,
A. Magerl, J. J. Rush, and J. M. Rowe. 15 Feb 86, 5p
Pub. in Physical Review B 33, n4 p2093 2097, 15 Feb 86.

Keywords: *Hydrogen, *Vanadium, *Niobium, *Tantalum, Intersititals, Defects, Reprints.

A report is made on measurements of the local modes of H in the transition metals V, Nb, and Ta with particular emphasis on low-concentration alloys. The excitations appear as very broad peaks in the neutron scattering spectrum even at a level of <1 at. % H, in contrast to the narrow density-of-states peaks normally expected for such interstitial defects. The lower vibration peak in NbH0.0055 reveals, within the alpha phase between 295 and 210 K, an unexpected continuous shift from 106 to 118 meV. Several possible mechanisms to explain these unusual observations are discussed and evaluated.

*601,235*
**PB86-231537** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Hafnium-Rhodium Constitution Diagram.**
Final rept.,
R. M. Waterstrat, and A. A. Giuseppetti. 1986, 9p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of the Less-Common Metals 119, p327-335 1986.

Keywords: Hafnium alloys, *Rhodium alloys, *Phase diagrams, Intermetallic compounds, Reprints.

A constitution diagram is presented for the Hf-Rh system. The liquidus rises to a maximum near the equiatomic composition and then falls rapidly with increasing hafnium content to a deep eutectic minimum at about 73 at.% Hf. The congruently melting equiatomic phase delta apparently transforms martensitically during cooling to one of several unidentified structures depending on the composition. The rhodium-rich phase gamma 1, based on a Cu3Au-type structure, exists over a rather broad composition range at high temperatures, but the range narrows at lower temperatures and approaches a composition away from the ideal stoichiometry. The intermediate phases eta-Hf2Rh and epsilon-Hf3Rh5 are stable over small composition ranges and form via peritectic reactions at about 1520 C and 2040 C respectively.

*601,236*
**PB86-238151** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Database Development under the ASM/NBS Program on Alloy Phase Diagrams.**
Final rept.,
K. J. Bhansali, D. F. Redmiles, J. L. Murray, and J. Sims. 1984, 15p
Proceedings of of National SAMPE Symposium and Exhibition, Reno, NV., April 3-5, 1984, v29 p1450-1464.

Keywords: *Phase diagrams, Alloys, *Data bases.

The ASM/NBS Phase Diagram Data Program addresses the need of the metals industry for up to date, critically assessed phase diagram data. Computerization is needed because of the sheer volume of phase diagram information currently being published. The scope of the computerization project goes beyond the treatment of text and digitization of figures, first because of the need for continuous update of critical assessments and second because of complex relationships among phase diagrams, crystallographic and thermodynamic data. Through a collaboration between the Metallurgy Division and the Center for Applied Mathematics, NBS is currently creating a prototype of the computerized phase diagram database. In the paper, evaluation of phase diagram data and the development of a prototype database are discussed.

*601,237*
**PB86-238342** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Vegard's Law.**
Final rept.,
L. H. Bennett, and A. J. McAlister. 1986, 2p
Pub. in Encyclopedia of Materials Science and Engineering, v7 p5241-5242 1986.

Keywords: *Solid solutions, Lattice parameters, Reprints, Vegard law.

Vegard's Law is an empirical rule which states that the lattice constant of a solid solution varies linearly as a function of concentration between the lattice constants of the components. It is found that metallic systems seldom, if ever, obey Vegard's Law exactly.

*601,238*
**PB86-238367** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Orientation Relationship between Precipitated Al9(Fe,Ni)2 Phase and Alpha-Aluminum.**
Final rept.,
L. Bendersky. Apr 85, 4p
Pub. in Metallurgical Transactions A 16A, n4 p683-686 Apr 85.

Keywords: *Aluminum alloys, Nickel containing alloys, Iron containing alloys, Phase, Orientation, Aluminum, Reprints, Rapid solidification.

The orientation relationship between Al9(Fe,Ni)2 precipitates and the FCC aluminum matrix in rapidly solidified Al-3.7, Ni-1.5 Fe (wt%) alloy has been determined. The precipitates are products of the supersaturated alpha-Al, decomposed by precipitation during continuous cooling immediately after solidification.

*601,239*
**PB86-241999** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**New Magnetic Phase Diagram of the Amorphous Pd-Fe-Si Ferroglass Alloy System.**
Final rept.,
R. B. Goldfarb, K. V. Rao, and H. S. Chen. 1986, 2p
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p111-112 1986.

Keywords: *Palladium alloys, Fron containing alloys, Silicon containing alloys, Phase diagrams, Reprints, Amorphous materials.

The magnetic phase diagram of amorphous Pd80-xFexSi20 is examined for 5 < or = x < or = 22. The authors use the peak in the imaginary component of ac susceptibility to determine the ferromagnetic-like to spin-glass transition temperatures T sub tg. It is found that the T sub tg curve is strongly field dependent and increases monotonically with increasing Fe concentration, even around x=22.

*601,240*
**PB87-105227** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Diffusion-Induced Grain-Boundary Migration in the Au-Ag System.**
Final rept.,
D. B. Butrymowicz, D. E. Newbury, D. Turnbull, and J. W. Cahn. 1984, 6p
Pub. in Scripta Metallurgica 18, n9 p1005-1010 1984.

Keywords: *Gold alloys, Silver containing alloys, Diffusion, Grain boundaries, Mass transport, Reprints.

Diffusion-induced grain boundary migration (DIGM) is a recently recognized phenomenon that leads to unexpected motion of grain boundaries. Vastly enhanced mass transport characterizes the low-temperature aspect of the phenomenon, since the grain boundaries provide easy paths for diffusion redistribution of atoms in the regions traversed at temperatures at which only grain boundary diffusion is significant has been observed to induce grain boundaries to migrate in a number of binary metal systems. At relatively low temperatures (where lattice diffusion is frozen out and where grain boundary diffusion prevails), migrating boundaries sweep across grains mixing in (or removing) solute. At these temperatures, no compositional changes occur except in regions through which the migrating boundaries pass, resulting in a discontinuous concentration range across the moving boundary. The Ag-Au system is investigated here with the aid of optical metallography, electron microprobe, and SEM.

*601,241*
**PB87-105235** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Cellular Microsegregation in Rapidly Solidified Silver-15 wt.% Copper Alloys.**
Final rept.,
L. A. Bendersky, and W. J. Boettinger. 1985, 4p
Pub. in Proceedings of the International Conference on Rapidly Quenched Metals (5th), p887-890 1985.

Keywords: *Silver alloys, Copper containing alloys, Microstructure, Silver alloy 15Cu, Rapid solidification.

Microstructural and microchemical analysis has been performed on Ag-15 wt% Cu alloys produced by electron beam melting with solidification velocities of 2.5, 12, and 18 cm/s. Cellular structures of the Ag-rich phase are produced with spacings of 0.8, 0.3, and 0.2 um, respectively. Intercellular regions contained fine eutectic at the lowest speed but only Cu-rich phase at the higher speeds. The composition within the cells was found to be nearly uniform and 12.5 plus or minus 1 wt% Cu. The uniformity and level of the Cu content within the cells are discussed.

*601,242*
**PB87-105243** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Effect of Rapid Solidification Velocity on Microstructure and Phase Solubility Extension in Nickel-Aluminum-Chromium (NiAl-Cr) Quasibinary Eutectic.**
Final rept.,
W. J. Boettinger, D. Shechtman, T. Z. Kattamis, and R. J. Schaefer. 1985, 4p
Pub. in Proceedings of the International Conference on Rapidly Quenched Metals (5th), p871-874 1985.

Keywords: *Nickel alloys, Aluminum containing alloys, Chromium containing alloys, Eutectics, Microstructure, Solubility, *Rapid solidification.

The transition from a two-phase rod-type eutectic microstructure to a single-phase Cr-supersaturated NiAl microstructure for the NiAl-Cr quasibinary eutectic composition is determined as a function of growth rate by electron beam melting and solidification scans. At growth rates below 1 cm/s the alloy exhibits a two-phase eutectic structure. Above 2.5 cm/s the structure solidifies as single phase Cr-supersaturated NiAl which subsequently decomposes spinodally.

*601,243*
**PB87-105250** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Environmental Effects on Titanium and Its Alloys.**
Final rept.,
H. B. Bomberger, D. A. Meyn, and A. C Fraker. 1985, 20p
Pub. in Proceedings of the International Conference on Titanium (5th), p2435-2454 1985.

Keywords: *Titanium, *Titanium alloys, Corrosion, Hydrogen embrittlement, Crack propagation.

Titanium and its alloys are exceptionally resistant to corrosion in natural environments and in many media in which other structural alloys including stainless steels are subject to unacceptable deterioration. This resistance is a consequence of a very thin, tenacious and durable natural oxide surface layer which confers passivity to a metal which would otherwise be rapidly consumed by contact with oxygen or water. However, titanium and its alloys are susceptible to several kinds of attack by environmental agents, especially under conditions where the natural oxide surface layer is disrupted and can not be quickly repaired. Such conditions include moderately high temperatures, strongly reducing corrosive environments, oxide-fluxing environments, plastic straining during exposure, high anodic potentials and low pH, or high cathodic potentials and low pH. Both the fundamental and practical aspects of environmental effects on titanium and its alloys are discussed.

*601,244*
**PB87-106365** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Neutron Powder Diffraction Studies of Two Uranium-0.75 wt. % Titanium Alloys.**
Final rept.,
C. S. Choi, and H. J. Prask. 1985, 4p
Pub. in Jnl. of Applied Crystallography 18, n3 p141-144 1985.

Keywords: *Uranium alloys, Tilanium containing alloys, Microstructure, Neutron diffraction, Line width, Particle size, Strains, Reprints.

The crystallographic and microstructural properties of depleted uranium alloys (0.75 wt.% Ti) with two different heat-treatments were studied by neutron powder diffraction methods. The crystal structures are essentially the same as that of pure alpha-uranium metal with somewhat different unit cell dimensions. The super saturated Ti impurity in the quenched sample is primarily substitutional. Diffraction lines of the quenched uranium alloy showed a clear strain broadening. The r.m.s. strain obtained from the broadening was 0.0019.

*601,245*
**PB87-114658** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.
**Elastically Induced Shape Bifurcations of Inclusions.**
Final rept.,
W. C. Johnson, and J. W. Cahn. 1984, 9p
Pub. in Acta Metallurgica 32, n11 p1925-1933 1984.

Keywords: *Inclusions, Shape, Reprints, Bifurcations.

Shape change transitions of elastically misfitting inclusions are predicted to occur when the inclusions are softer than the matrix. Below the size where the transition occurs, the shape is dictated by minimizing interfacial energy without regard to the elastic contribution. The transition is to a lower symmetry shape that is influenced by the elastic contribution. Transitions analogous to a second-order phase transition are predicted for an isotropic two-dimensional or plane-strain case, while transitions analogous to first-order phase transitions are predicted for an isotropic three-dimensional case.

*601,246*
**PB87-118576** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Magnetic Excitations in Chromium II.**
Final rept.,
B. H. Grier, G. Shirane, and S. A. Werner. 1985, 10p
Pub. in Physical Review B: Condensed Matter 31, n5 p2892-2901 1985.

Keywords: *Chromium, Magnetic properties, Magnons, Neutron scattering, Reprints.

Neutron scattering measurements on pure chromium metal have been performed under various conditions of experimental resolution, energy transfer, temperature and magnetic field. The temperature and energy dependence of the commensurate-diffuse scattering surrounding the (001) point in reciprocal space has been followed from the spin flip temperature (T sub sf = 122 K) to temperatures as high as 700 K, well above the Neel point T sub N = 312 K). Magnetic correlations extending over 11 bcc unit cells persist to these high temperatures. The spectral width of the magnetic scattering is found to increase rapidly with temperature above T sub N. The importance of the commensurate-diffuse modes of excitation in the disappearance of the long-range ordered SDW state at T sub N is discussed. The magnetic field dependence of the excitations in the transversely polarized SDW Phase has been investigated and found to be absent.

*601,247*
**PB87-119145** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Semi-Elliptical Surface Flaw EC (Eddy Current) Interaction and Inversion: Experiment.**
Final rept.,
J. C. Moulder, J. C. Gerlitz, B. A. Auld, and S. Jefferies. 1986, 8p
Sponsored by Ames Lab., IA.
Pub. in Review of Progress in Quantitative Nondestructive Evaluation 5A, p395-402 1986.

Keywords: *Cracks, *Aluminum alloys, *Titanium alloys, Eddy current tests, Nondestructive tests, Fatigue(Materials), Reprints, *Flaws, Notches.

Eddy current flaw signals were measured for a series of fatigue cracks and semi-elliptical, electrical-discharge machined notches in aluminum and titanium alloys. Absolute magnitude and phase of the change in eddy current probe impedance were determined by scanning the probe along the length of the flaw and measuring the probe impedance with a digital impedance analyzer. Both air-core and ferrite-core probes were used. Differences in the flaw signals from nominally identical air-core probes were traced to different magnetic field intensities of the probes. Experimental results are compared with flaw profiles calculated using a finite difference numerical model developed at Stanford University, which is described in a companion paper.

*601,248*
**PB87-122487** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Automated Fatigue Crack Growth Rate Test System.**
Final rept.,
Y. W. Cheng, and D. T. Read. 1985, 11p
Sponsored by Minerals Management Service, Reston, VA., and Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in American Society of Testing and Materials Special Technical Testing Publication 877, p213-223 1985.

Keywords: *Crack propagation, *Fatigue(Materials), Fatigue tests, Cracking(Fatigue), Nondestructive tests, Reprints.

An automated fatigue crack growth rate (FCGR) test system has been developed that can be used for tests of constant-load-amplitude FCGR above 10 to the -8th power m/cycle (ASTM Test Method for Constant-Load-Amplitude Fatigue Crack Growth Rates Above 10 to the -8th power m/Cycle(E647-83)) at normal (approx. 10 Hz) or low (approx. 0.1 Hz) cyclic frequencies and for tests of near-threshold and variable-load-amplitude FCGR. The test system consists of a minicomputer, a programmable arbitrary waveform generator, a servo-hydraulic test frame, and a programmable digital oscilloscope. The crack length is measured using the compliance technique; the FCGR and the stress-intensity factor range are calculated and plotted automatically during the test.

*601,249*
**PB87-122503** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

**Nickel and Nitrogen Alloying Effects on the Strength and Toughness of Austenitic Stainless Steels at 4 K.**
Final rept.,
R. P. Reed, P. T. Purtscher, and K. A. Yushchenko. 1986, 8p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Advances in Cryogenic Engineering 31, p43-50 Sep 86.

Keywords: *Austenitic stainless steels, *Tensile strength, Low temperature tests, Tensile properties, Cryogenics, Nickel alloys, Reprints, *Fracture toughness, Nickel nitrogen alloys.

The tensile strength and fracture toughness at 4 K were studied as a function of Ni (6-15 wt.%) and N (0.90-0.28 wt.%) contents for eight austenitic stainless steels. Results indicate that Ni increases the tensile yield strength and decreases the fracture toughness, Klc(J), and Ni has little effect on tensile yield strength but increases the fracture toughness. The temperature dependence of the yield strength is given by sigma(sub y) = sigma(sub o) e(sup (-) AT), where sigma(sub o) is the yield strength at O K, and A is the slope of ln sigma(sub y) vs. T. The parameter A is proportional to the stacking fault energy. Lower Ni alloys exhibited brittle facets on fracture surfaces. The quality index, a new parameter = sigma(sub y) K(sub Ic) (J), relates to the capacity of the alloy to achieve greater strength or toughness, but not at the expense of the other parameter. Nickel alloying increases the quality factor; nitrogen has little effect.

*601,250*
**PB87-122511** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Sizing Planar Flaws in Weldments Using Low-Frequency EMATs (Electromagnetic-Acoustic Transducers).**
Final rept.,
R. E. Schramm, and T. A. Siewert. 1986, 8p
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.
Pub. in Second Half of the Proceedings of Annual Review of Progress in Quantitative Nondestructive Evaluation (12th), Williamsburg, VA., June 23-28, 1985, v5B p1705-1712 1986.

Keywords: *Weld defects, Weldments, Nondestructive tests, Ultrasonic tests, Transducers.

The report describes a significant improvement in flaw sizing capability using electromagnetic-acoustic transducers (EMATs) operating near 0.5 MHz. Previous work demonstrated the use of backscattered signals for determining flaw depths in the range of 0.5 to 3 mm; for deeper flaws the signal saturated. In the new procedure, a second receiver measures the forward-scattered signal transmitted through the weld. Using the backscattered to forward scattered ratio as a sizing parameter has extended the depth sizing range to at least 10 mm. Artificial flaws were used to generate a calibration curve used to size real lack-of-penetration weld flaws in 16-mm thick ferritic steel plates. True flaw depths, as determined by metallography, were in very good agreement with those determined by the ultrasonic measurements.

*601,251*
**PB87-122560** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Roughening of Low-Angle Grain Boundaries.**
Final rept.,
C. Rottman. 1986, 5p
Pub. in Physical Review Letters 57, n6 p735-738, 11 Aug 86.

Keywords: *Grain boundaries, Crystal dislocations, Interfaces, Melting, Reprints.

The possibility of roughening in low-angle grain boundaries is investigated. By exhibiting an analogy between grain-boundary steps which do not have long-range strain and steps on solid surfaces, the author argues that a grain-boundary roughening transition, of the same type as for solid surfaces, is possible.

*601,252*
**PB87-122842** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

**Influence of Thermal Processing on Fatigue Crack Initiation and Propagation of Ti-4.5Al-5Mo-1.5Cr.**
Final rept.,
C. M. Gilmore, M. A. Imam, A. C. Fracker, S. H. Yang, and A. C. Van Orden. 1985, 8p
Pub. in Proceedings of the International Conference on Titanium (5th), Washington, DC., v4 p2091-2098 1985.

Keywords: *Titanium alloys, Heat treatment, Cracking(Fracturing), Fatigue(Materials), Martensite, Crack propagation, Mechanical properties, Microstructures, Titanium alloy 4.5 Al 1.5 Cr 5 Mo.

The effects of thermal treatment on the microstructure and mechanical behavior of the Al-.Cr (-5Mo-1.5Cr (Corona 5) alloy were studied. The temperature range studied was 870C - 965C. Fatigue crack growth rates were not significantly affected by the presence of metastable beta Ti and its strain induced transformation to martensite. Fatigue crack initiation and fatigue life are affected by the presence of a metastable beta phase.

*601,253*
**PB87-127940** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.
**Optical Measurement of the Roughness of Sinusoidal Surfaces.**
Final rept.,
T. V. Vorburger, D. E. Gilsinn, F. E. Scire, M. J. McLay, and C. H. W. Giauque. 1986, 13p
Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center.
Pub. in Wear 109, p15-27 1986.

Keywords: *Surface roughness, Roughness, Scattering, Metal working, Reprints.

Results are presented for optical scattering measurements of six sinusoidal surfaces with a roughness average R(sub a) ranging from 0.3 to 3 micrometers and wavelengths ranging from 40 to 800 micrometers. The probe was an He-Ne laser beam with a 0.6328 micrometers wavelength. The multipeaked scattering distributions were fitted by a straightforward phase screen integral to find the amplitude and spatial frequency parameters that then yielded results for R(sub a) and the spatial wavelength for each surface. The agreement with the comparable parameters as measured by a stylus instrument is excellent. This leads to the observation that optical scattering with visible light in conjunction with a straightforward optical theory can yield accurate measurements of roughness parameters provided that the surface roughness itself can be accurately modeled with appropriate a priori knowledge and provided that the surface slopes and heights are in the ranges represented by these sinusoidal surfaces.

*601,254*
**PB87-127965** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Interaction of Line Singularities Near a Crack Tip and Their Application to Surface Stresses at Cracks.**
Final rept.,
R. Thomson, T. J. Chuang, and I. H. Lin. 1985, 8p
Pub. in Predictive Capabilities in Environmentally Assisted Cracking, p187-194 1985.

Keywords: *Crack propagation, Cracking(Fracturing), Dislocations(Materials), Ductility, Stresses, Reprints.

An elastic analysis of line singularities interacting with a crack is developed. The line singularities simulate the action of surface stresses which are present on all open surfaces, and which can be modified by adsorbtion of foreign chemical species on the cleavage surface near the crack tip. Results are presented showing that shielding k-fields at the crack are generated by anti-symmetric line dipoles. A symmetrical line dipole interacts only with other symmetrical line dipoles. When dislocations are included near the crack tip, it is found that under elastic conditions for a slit crack, dipoles of both kinds exert forces on the dislocation and can modify the ductility of materials.

*601,255*
**PB87-128021** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

**Low Temperature Deformation of Copper and an Austenitic Stainless Steel.**
Final rept.,
R. P. Reed, and R. P. Walsh. 1986, 10p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Advances in Cryogenic Engineering 32, p303-312 1986.

Keywords: *Deformation, *Copper, *Austenitic stainless steels, Cryogenics, Low temperature tests, Tensile properties, Stress strain diagrams, Reprints, Steel AISI 310, Copper 10Z alloy.

The tensile-deformation characteristics and effect of strain rate were studied on relatively pure CDA 102 Cu and solid-solution-strengthened AISI 310. Tensile strain rate was varied between two orders of magnitude (0002 ;0.00005/s) at temperatures ranging from 4 to 295 K. Tensile stress-strain-hardening curves were determined for these temperatures. The effect of strain-rate changes on tensile flow strength was measured from strains near 0.002 (yield strength) to over 0.300. The data reflect three distinct ranges of face-centered cubic, polycrystalline plastic deformation, which have different characteristics depending on solute content.

*601,256*
**PB87-128799** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Ultrasonic Determination of Principal-Stress Differences for a Slightly Anisotropic Residual Stress Specimen.**
Final rept.,
A. V. Clark, and J. C. Moulder. 1986, 11p
Pub. in Proceedings of Symposium on Nondestructive Evaluation (15th), San Antonio, TX., April 23-25, 1985, p260-270 1986.

Keywords: *Dynamic structural analysis, *Aluminum alloys, Nondestructive tests, Stresses, Structural analysis, Ultrasonic tests, Anisotropy, Texture, Acoustical birefringence.

The authors have used the acoustical birefringence technique to measure the difference of principal stresses in a specimen in a well-characterized state of residual stress. In this technique, the difference in aribal times of orthogonally polarized SH-waves (acoustical birefringence) is measured and then related to stress. Because the specimen is slightly anisotropic, it exhibits birefringence even in the unstressed state; in the specimen this initial birefringence, Bo, can be as large as (or larger than) that caused by stress. The authors used noncontacting EMATs, which allowed the measurements to be made quickly without introducing errors in arrival time due to couplant thickness variations. Experiments were first performed with the EMATs in the pitch-catch configuration, the authors found good agreement with theoretical predictions of the principal-stress differences for the shrink-fit aluminum alloy specimen.

*601,257*
**PB87-128955** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Macrocrack-Dislocation Pile-up Interactions.**
Final rept.,
I. H. Lin. 1986, 11p
Pub. in Materials Science and Engineering 81, p325-335 1986.

Keywords: *Dislocations, *Loading(Mechanics), Stresses, Fracture toughness, Crack propagation, Reprints, *Microcracks.

In this paper the elastic interaction between a macrocrack and an excess double-ended pile-up under general loading is developed. The quantitative prediction of local stress intensity factors at the macrocrack tip and the blocked leading dislocations and the forces on each singularity are derived. These physical quantities are shown as functions of the dislocation-free zone, the pile-up size, the number and the sign of excess dislocations in the pile-up and the applied stress intensity factors. Results are presented which show that Newton's third law is satisfied between the macrocrack tip and blocked leading dislocations. It is found that a macrocrack tip is always antishielded by a pure double-ended pile-up. The elastic interaction developed in the paper is very general and four important pile-up limits are treated in the paper.

*601,258*
**PB87-128989** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Elastic-Plastic Response of Tensile Panels Containing Short Center Cracks.**
Final rept.,
R. H. Dodds, and D. T. Read. 1984, 10p
Sponsored by Naval Sea Systems Command, Washington, DC.
Pub. in Proceedings of 1984 Pressure Vessel and Piping Conference and Exhibition, San Antonio, TX., June 17-21, 1984, p25-34.

Keywords: Cracking(Fracturing), Panels, Finite element analysis, Fracture properties, Deformation, *J integrals.

The finite element method (FEM) is used to predict applied J-integral values in highly strained tensile panels containing short center cracks. Experimental J-values are obtained by integrating strain and displacement quantities measured along an instrumented contour. FEM plane stress predictions for J-values and crack mouth opening displacements are much larger than experimentally measured values for short cracks ($a/W < 0.05$). Large geometry changes near the crack tip are demonstrated to have a negligible effect on the FEM J-values. The introduction of a small stiffened zone near the crack tip using an overlay of plane strain elements brings FEM J and CMOD values into close agreement with experimental values. For longer crack lengths, conventional plane stress FEM solutions are adequate to predict J and CMOD values.

*601,259*
**PB87-132767** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Absolute Ultrasonic Determination of Stresses in Aluminum Alloys.**
Final rept.,
A. V. Clark, and J. C. Moulder. 1986, 11p
Pub. in Review of Progress in Quantitative Nondestructive Evaluation 5B, p1449-1459 1986.

Keywords: *Stresses, *Aluminum alloys, Nondestructive tests, Reprints, Acoustic birefringence, Ultrasonics.

Ultrasonic methods are currently being investigated as a means of nondestructive stress measurement. The authors have considered various methods to obtain individual stress components using shear-horizontal (SH-) waves in slightly anisotropic (textured) structural components. For rolled aluminum alloy plates, there are typically three two-fold material symmetry axes. Referring stresses to these axes, the authors find that different methods of absolute stress determination must be used, depending upon whether or not the principal stress and material symmetry axes coincide. Furthermore, the presence of texture causes an initial birefringence; the birefringence is defined as the normalized difference in phase velocity of orthogonally polarized, pure-mode SH-waves.

*601,260*
**PB87-132775** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Ultrasonic Techniques for Residual Stress Measurement in Thin Welded Aluminum Alloy Plates.**
Final rept.,
A. V. Clark, J. C. Moulder, R. E. Trevisan, T. A. Siewert, and R. B. Mignogna. 1986, 12p
Sponsored by Naval Research Lab., Washington, DC.
Pub. in Review of Progress in Quantitative Nondestructive Evaluation 5B, p1461-1472 1986.

Keywords: *Metal plates, *Aluminum alloys, *Stresses, Welding, Ultrasonic tests, Nondestructive tests, Reprints, Acoustic birefringence.

Thin aluminum alloy plates were single-pass butt-welded to produce a state of plane residual stress. Strain gages bonded to the plates prior to welding were used to measure the residual stresses. Residual stresses were also measured ultrasonically by three different methods. The acoustic birefringence technique was used to measure the principal stress difference, delta sigma, near the center of the welded plates. Noncontacting EMATs were used to measure arrival times of SH-waves before and after welding. Near the plate edges, a shear stress sigma (xy) exists. The gradient of sigma (xy) was measured with the acoustic birefringence technique and substituted into the stress-equilibrium equation to calculate the normal stress. Values obtained were within about 20 MPa of the strain gage data.

*601,261*
**PB87-135216** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Extraction Replica Method for the Study of Surface Films.**
Final rept.,
L. K. Ives. 1985, 4p
ASLE (American Society of Lubrication Engineers) Transactions 28, n1 p87-90 1985.

Keywords: *Surfaces, *Thin films, Wear, Surface chemistry, Substrates, Iron oxides, Iron sulfides, Reprints, *Extraction replica.

An extraction replica method is described by means of which thin solid films on worn surfaces may be removed from selected areas for examination in the transmission electron microscope. A scratch or several scratches are made on the worn surface with a pointed stylus. Displaced or loosened fragments of material are removed by means of a plastic extraction replica. After subsequent processing of the replica, sufficiently thin fragments can then be examined by transmission electron microscopy, electron diffraction and the allied methods of x-ray energy dispersive analysis and electron energy loss spectroscopy. The latter two methods permit the determination of chemical composition which can then be correlated with crystallographic and microstructural observations. Application of the scratch extraction replica method is illustrated with examples of films removed from worn steel specimens lubricated with paraffinic mineral oil, mineral oil with 1 wt.% ZDP, and with a formulated reference motor oil.

*601,262*
**PB87-135224** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Equilibrium Solute Concentration Surrounding Elastically Interacting Precipitates.**
Final rept.,
W. C. Johnson, and P. W. Voorhees. 1985, 11p
Pub. in Metallurgical Transactions A-Physical Metallurgy and Materials Science 16, n3 p337-347 1985.

Keywords: *Precipitates, *Concentration(Composition), Thermodynamics, Elasticity, Metallurgy, Solutes, Stress analysis, Reprints.

Elastically induced equilibrium solute concentration profiles surrounding isolated and two elastically interacting precipitates are determined under the conditions of an applied shear and tensile stress, as well as an isotropic stress-free transformation strain. The self consistent open-system elastic constants approach is employed to account explicitly for the coupling between the stress and concentration fields. Substantial concentration changes are predicted near the surfaces of the particles which can easily exceed 50%. With self consistency to first-order in the concentration change, no net solute enhancement is observed surrounding isolated particles while net solute segregation is observed for elastically interacting particles.

*601,263*
**PB87-136685** PC **A06**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.
**Institute for Materials Science and Engineering, Metallurgy: Technical Activities 1986.**
Annual rept.
Oct 86, 105p NBSIR-86/3438
See also PB86-196771.

Keywords: *Metallurgy, Processing, Metals, Alloys, Nondestructive tests, Chemical properties, Mechanical properties, Corrosion, Wear, Electrodeposition, Magnetic materials, Technical activities.

The report summarizes the FY 1986 activities of the Metallurgy Division of the National Bureau of Standards. The research centers upon the structure-processing-properties relations of metals and alloys, and on the methods of their measurement. Efforts comprise studies of synchrotron radiation research for materials characterization, metallurgical processing, wear and mechanical properties, chemical metallurgy, corrosion and protection of metals, electrodeposition, nondestructive characterization, and magnetic materials. The work herein described includes three cooperative data programs with American professional societies and industry: the American Society for Metals-NBS Alloy Phase Diagram Program, the National Association of Corrosion Engineers-NBS Corrosion Data Program, and the American Iron and Steel Institute-NBS Steel Sensor Program.

## Plastics

*601,264*
**PB86-160769** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Response of Radiochromic Film Dosimeters to Gamma Rays in Different Atmospheres.**
Final rept.,
W. L. McLaughlin, J. C. Humphreys, and C. Wenxiu. 1985, 13p
Pub. in Radiation Physics and Chemistry 25, n4-6 p793-805 1985.

Keywords: *Polymer films, *Plastics, *Dosimetry, *Radiation damage, *Gamma rays, Polystyrene, Polyvinyl chloride, Nylon, Irradiation, Stability, Reprints.

The high-dose gamma ray response (1000-500,000 Gy) of radiochromic film dosimeters, with ten kinds of plastic matrices (polychlorostyrene containing 1 or 25% Cl, polybromostyrene containing 2 or 43% Br, nylon, polyvinyl chloride, cellulose triacetate, and an aromatic polyamide) were investigated when irradiated under certain conditions in vacuum and in different atmospheres (air, oxygen, nitrogen, and nitrous oxide). In addition, the stability of the films was studied for storage periods up to one month after irradiation under these conditions. The responses and stabilities of the polyhalostyrene and nylon films were only slightly affected by the different atmospheres of irradiation, but there were marked differences of response for the other film types. Emphasis must be given to differences in atmospheric conditions encountered by dosimeters in practical industrial situations, which may cause marked differences in ultimate response factors.

*601,265*
**PB86-160777** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Radiochromic Dye Dosimetry Using Triphenylmethane Leucocyanides in Nylon or Polyvinyl Butyral.**
Final rept.,
W. L. McLaughlin, and J. C. Humphreys. 1984, 28p
Pub. in Proceedings of High Dose Standardization and Intercomparison for Industrial Radiation Processing, Munich, Germany, November 8-11, 1983, p209-236 1984.

Keywords: *Polymer films, *Dosimetry, *Cobalt, *Nylon, Gamma radiation, Temperature, Vacuum environment, Stability, Humidity, Temperature, *Poly(butyral/vinyl), *Radiochromic dye dosimetry.

The use of commercially-available radiochromic plastic films (nylon or polyvinylbutyral) containing the leucocyanide of hexa (hydroxyethyl) pararosaniline is well established in radiation processing dosimetry (dose range: (10-100,000 Gy), especially for (60)Co gamma-ray applications. These thin-film systems when analyzed by spectrophotometry provide a convenient and routine means of dose assessment and dose-distribution mapping, as long as they are properly calibrated in standard gamma-ray fields and as long as suitable corrections are made for systematic error. In the present work, the following contributions to uncertainty in making absorbed dose evaluations with radiochromic film dosimeters were studied: variations in absorbed dose rate, photon energy, temperature, relative humidity, vacuum, and presence of gases other than air (oxygen, nitrogen, nitrous oxide) during irradiation and during storage. These influences on radiochromic dosimeter response and stability have been studied in detail experimentally, and suggestions are made for minimizing such uncertainties in practice.

*601,266*
**PB86-160785** Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Plastic Film Materials for Dosimetry of Very Large Absorbed Doses.**
Final rept.,
W. L. McLaughlin, A. Miller, F. Abdel-Rahim, and T. Preisinger. 1985, 20p
Pub. in Radiation Physics and Chemistry 25, n4-6 p729-748 1985.

Keywords: *Polymer films, *Plastics, *Radiation damage, *Dosimetry, Dosage, Absorption, Dyeing, Polyethylene terephthalate, Polyethylene, Polyvinyl chloride, Polystyrene, Reprints, Vinylidene fluoride resins.

Most plastic films have limited response ranges for dosimetry because of radiation-induced brittleness, degradation, or saturation of the signal used for analysis (e.g. spectrophotometry) at high doses. There are, however, a few types of thin plastic films showing linearity of response even up to doses as high as 2,000,000 Gy (200 Mrad) without severe loss of mechanical properties. Among many candidate film types tested, those showing such resistance to radiation damage and continued response at such high doses are polyethylene terephthalate, high-density polyethylene, dyed polyvinylchloride, polystyrene, dyed and undyed polyhalostyrenes, dyed aromatic polyamides, and polyvinylidene fluoride. Although most of these systems have fairly stable absorption spectra after irradiation, tests of dependence on dose rate and on temperature during irradiation show that only polystyrene and some of the polyhalostyrenes have essentially rate-indepent and moderately temperature-dependent responses to such large doses of ionizing radiation. While radiation-induced optical absorption in the ultraviolet for polystyrene is unstable following irradiation, thus leading to an intrinsic low-intensity rate dependence, the dyed polychlorostyrenes show essentially the same response to radiation-processing gamma-ray fields and to very high-intensity electron beams, and a relatively stable absorption spectrum at wavelengths for dosimetry analysis in the visible spectral region of about 430 nm.

*601,267*
**PB86-183605** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Shielding Effectiveness Measurements of Plastics,**
J. W. Adams, and E. J. Vanzura. Jan 86, 33p NBSIR-85/3035

Keywords: *Plastics, *Electromagnetic shielding, Effectiveness, Measurement.

Measurement of shielding effectiveness (SE) of plastic materials may give serious problems due to the insulating nature of many plastics. A method of making these measurements using a flanged coaxial holder overcomes these limitations.

*601,268*
**PB86-186681** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Generation of Hydrogen Cyanide from Flexible Polyurethane Foam Decomposed Under Different Combustion Conditions.**
Final rept.,
B. C. Levin, M. Paabo, M. L. Fultz, and C. S. Bailey. 1985, 10p
Pub. in Fire and Materials 9, n3 p125-134 1985.

Keywords: *Polyurethane resins, *Hydrogen cyanide, *Combustion products, Flammability testing, Fire resistant materials, Ignition, Decomposition, Chemical analysis, Chars, Reprints.

Experimental thermal conditions conducive to the production of high levels of hydrogen cyanide (HCN) from flexible polyurethane foam were determined. In these experiments the material was exposed to relatively low-temperature non-flaming oxidative conditions for a short time period, during which a char was formed. Further heating of the char to temperatures above 500 deg C generated the increased HCN levels. Upon exposure to the same two-step decomposition process, a fire-retarded flexible polyurethane foam produced twice as much char and twice as much HCN.

*601,269*
**PB86-190667** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Influence of Strain Deformation on the Solubility of Ethyl Acetate Vapor in Poly(vinylidene fluoride).**
Final rept.,
J. C. Phillips, A. Peterlin, and P. F. Waters. 1984, 7p
Pub. in Jnl. of Polymer Science, Polymer Physics Edition 22, n10 p1719-1725 1984.

Keywords: *Plastic deformation, *Solubility, *Ethyl acetate, *Vinylidene fluoride polymers, Deformation, Strains, Plastic flow, Transport properties, Vinyl plastics, Reprints.

The degree to which a polymer film develops plastic flow depends largely on the total strain epsilon and the elongation time t sub h. The magnitude and the time dependency of the elastic component epsilon sub e of the total deformation are controlling factors, respectively, in the solubility and diffusion processes. The plastic deformation epsilon sub p seems not to contribute to the transport properties. The non-linearity in solubility due to epsilon may be conveniently handled. In the study, the solubility of Ethyl Acetate vapor in Polyvinylidene Fluoride was determined as a function of pressure and total elongation at 30 deg C. These results tend to indicate that the strain magnitude and time dependency of the component deformations play an important role in transport behavior.

*601,270*
**PB86-191426** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Creep and Recovery Behavior of Ultra-High Molecular Weight Polyethylene in the Region of Small Uniaxial Deformations.**
Final rept.,
L. J. Zapas, and J. M. Crissman. 1984, 6p
Pub. in Polymer 25, n1 p57-62 1984.

Keywords: *Polyethylene, *Creep properties, *Stress relaxation, *Viscoplasticity, Constitutive equations, Recovery, Reprints, Stress-strain relationships.

The creep and recovery behavior of an ultra high molecular weight polyethylene (UHMWPE) has been studied in the region of small uniaxial deformations. At deformations as small as .0005 the stress-strain behavior is non-linear and the recovery cannot be described by a theory of fading memory. A new one dimensional constitutive relation is presented which describes quantitatively the multistep creep and recovery behavior of the material in the case where the specimens were not mechanically preconditioned. The multistep in strain stress relaxation behavior of the UHMWPE has also been investigated for the case in which the second step in strain is approximately half the magnitude of the first step. Calculations of the strain necessary in order to give the observed stress in a two step stress-relaxation experiment have been made assuming that the stress-relaxation experiment can be represented by a series of multistep creep experiments where in each step the stress is adjusted so as to maintain a constant deformation.

*601,271*
**PB86-191459** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Aspects of the Characterization of Ultra-High Molecular Weight Polyethylene.**
Final rept.,
H. L. Wagner, and J. G. Dillon. 1984, 5p
Pub. in Polym. Mater. Sci. Eng. 50, p53-57 1984.

Keywords: *Polyethylene, *Molecular weight, Chemical properties, Viscosity, Transport properties, Reprints, Characterization.

The measurement of molecular weight and molecular weight distribution of ultra high molecular weight polyethylene (UHMWPE) is essential for specification and control. However, there are many problems with conventional characterization techniques such as dilute solution viscosity, light scattering, and size exclusion chromatography (SEC or GPC). This is further complicated by its poor solubility and sensitivity to degradation. The viscosity is shear rate dependent, requiring that measurements be made in a low shear rate viscometer. The exclusion limit of presently available commercial SEC columns appears to be too low for UHMWPE, and in addition the polymer may undergo degradation during the run. Therefore, to determine the molecular weight distribution, a sample of commercial UHMWPE was subjected to a hydrodynamically induced crystallization to yield 10 fractions with limiting viscosity numbers ranging from 9 to 50 dL/g. Assuming that the Mark-Houwink relation for low molecular weight polyethylene holds for these higher molecular weight fractions, an integral distribution was obtained with molecular weights as high as 1 x 10 to the 7th power.

*601,272*
**PB86-201035** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Necking of Semicrystalline Polymers in Tension.**
Final rept.,
L. J. Zapas, and J. M. Crissman. 1984, 18p
Pub. in Proceedings of Workshop Orienting Polymers, Minneapolis, MN., March 21-26, 1983, p46-63.

Keywords: *Necking, *Polypropylene, *Polyethylene, Tensile properties, Axial strain, Axial stress, Stability, Polymers, *Semicrystalline polymers.

The phenomenon of necking under various uniaxial stress and strain histories has been studied for several semicrystalline polymers. A rather detailed presentation is given on a quenched isotactic polypropylene and comparison of the experimental results is made to the Bernstein and Zapas theory on the instability of viscoelastic bars. Data are also presented for various polyethylenes under constant load uniaxial deformations, and diagrams showing the locus of points in strain and time at which necking occurs are given.

*601,273*
**PB86-208477** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Differences in PMMA Degradation Characteristics and Their Effects on Its Fire Properties.**
Final rept.,
T. Kashiwagi, A. Inaba, and J. E. Brown. 1986, 11p
Pub. in Proceedings of International Symposium on Fire Safety (1st), Gaithersburg, MD., October 7-11, 1985, p483-493 1986.

Keywords: *Polymethyl methacrylate, Fire tests, Degradation, Fire studies.

Thermal degradation and thermal oxidative degradation characteristics of Plexiglas G and Lucite were determined using thermogravimetry. The results show that degradation rate of Plexiglas G is sensitive to gas phase oxygen but that of Lucite is much less so. Comparison of derivative thermogravimetry curves between the two samples indicates that at low temperatures Plexiglas G is more stable with respect to degradation in nitrogen. Lucite is initially more stable with respect to degradation in air than is Plexiglas G. A similar trend was observed in a nonflaming gasification study using external radiative heating. It appears that the chemical nature of the degradation processes of the two samples is the same for slow heating thermogravimetry and for more rapid heating (gasification study) simulating a fire environment.

*601,274*
**PB86-209954** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Compatibility of Hydrogenated and Deuterated Polystyrene.**
Final rept.,
H. Yang, R. Stein, C. Han, B. Bauer, and E. Kramer. 1986, 4p
Sponsored by National Science Foundation, Washington, DC. Div. of Materials Research, and Massachusetts Univ., Amherst. Materials Research Lab.
Pub. in Polymer Communications 27, p132-135 May 86.

Keywords: *Compatibility, Hydrogenation, Reprints, *Polystyrene, Correlation length, Polymer blends, Neutron scattering.

A 50/50 blend of deuterated polystyrene (PSD,Mw =255 times 10 to the 3rd power) and polystyrene (PSH, Mw =233 times 10 to the 3rd power) was studied by small-angle neutron scattering (SANS) for its interaction parameter, x/vo, correlation length, and susceptibility, S(q=0) at various temperatures. The interaction parameter x/vo has a value of less than 10-6, which is within the error limit of being zero in the measurement temperature range. The error bound cannot exclude the possibility of an upper critical solution temperature (UCST). However, this UCST, if it exists, will be well below the glass transition temperature for any PSD/PSH blends with reasonable molecu-

lar weight. Phase separation of PSD/PSH blends does not occur under common experimental conditions and phase separation of isotopically labelled polymers is not a general phenomenon but a specific property of individual polymers.

*601,275*
**PB86-230802** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Model Describing the Steady-State Gasification of Bubble-Forming Thermoplastics in Response to an Incident Heat Flux.**
Final rept.,
I. S. Wichman. Feb 86, 13p
Pub. in Combustion and Flame 63, nl-2 p229 Jan-Feb 86.

Keywords: *Thermoplastic resins, *Gasification, Bubbles, Heat flux, Reprints.

A theoretical model is developed to describe the in-depth effect of bubbles on the steady-state transport of volatile gases from the surface of a thermoplastic material subjected to an incident conductive heat flux. In the model the effect of the bubbles on the surrounding liquid is felt through the bubble number distribution function, n, which appears in the equations for conservation of mass, momentum, species, and energy in the melt. The equation describing the evolution of n includes the effects of bubble growth, convection, and nucleation.

*601,276*
**PB86-232766** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Tensile, Compressive, and Shear Properties of Polyurethane Foam at Low Temperatures.**
Final rept.,
J. M. Arvidson, and L. L. Sparks. 1982, 10p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in Advances in Cryogenic Engineering 28, p289-298 1982.

Keywords: *Foam, *Polyurethane resins, Low temperature tests, Mechanical properties, Cryogenics, Tension, Compressive strengths, Elastic properties, Shear strength, Yield strength, Modulus of elasticity, Reprints.

Polyurethane foam, having a density of 32 kg/cu m, was tested at 295, 111, 76, and 45K in helium gas. The material properties reported are Young's modulus, proportional left, yield strength (at 0.2% offset), tensile and compressive strengths, and elongation (elastic and plastic). To perform these tests a new apparatus was developed. The apparatus permits tension, compression, and shear testing of materials at any temperature ranging from 295 to 4K. The system also incorporates a concentric, overlapping-cylinder capacitance extensometer which is highly sensitive and linear in output.

*601,277*
**PB87-108114** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Effects of Weak Linkages on the Thermal and Oxidative Degradation of Poly(methyl methacrylates).**
Final rept.,
T. Kashiwagi, A. Inaba, J. E. Brown, K. Hatada, and T. Kitayama. 1986, 9p
Pub. in Macromolecules 19, p2160-2168 1986.

Keywords: *Polymethyl methacrylate, Thermal degradation, Oxidation, Leakage, Nitrogen, Air, Thermogravimetry, Polymerization, Reprints.

The thermal and oxidative degradation mechanisms of poly(methyl methacrylate) (PMMA) were studied in atmospheres of nitrogen and air by thermogravimetry using various specially polymerized samples. Thermal degradation of PMMA polymerized with a free radical method proceeds in three steps of weight loss: the least stable step is initiated by scissions of head-to-head linkages, the second step by scissions at the chain-end initiation from vinylidene ends, and the most stable step by random scission within the polymer chain. There are no significant differences seen in the thermal or oxidative degradation of PMMA polymerized with the free radical method between azobis(isobutyronitrile) and benzoyl peroxide as the initiators. Gas-phase oxygen traps radicals resulting from chain scissions at head-to-head linkages. No weight loss observed from this step in air. Similarly, oxygen traps radicals generated by end initiation, but it is not as effective as for the case of head-to-head linkages. Possible mechanisms for end initiation and oxidative termination of radicals initiated from scission at the head-to-head linkages are discussed.

*601,278*
**PB87-108130** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
**Workshop Proceedings: Morphology of Polyethylene and Cross-Linked Polyethylene.**
Final rept.,
M. G. Broadhurst, F. A. Khoury, A. J. Bur, and G. T. Davis. Nov 81, 33p
Sponsored by Electric Power Research Inst., Palo Alto, CA.
Pub. in Proceedings of Workshop on Morphology of Polyethylene and Cross-Linked Polyethylene, Gaithersburg, MD., March 31-April 1, 1981, 33p.

Keywords: *Polyethylene, *Meetings, *Electrical insulation, Morphology, Electron microscopy, Crosslinking, Power transmission lines, Aging.

The report summarizes the proceedings of a workshop on the morphology of extruded polyethylane power cable insulation. The purpose of the workshop was to review the state-of-the-art of morphological studies of cross-linked and uncross-linked polyethylene, to determine the potential relevance of the parameter in aging of these electrical insulation materials, and to arrive at suggestions for future work in the area. A major concern which developed during the workshop was that some of the features shown and reported in the literature might be artifacts resulting from the techniques used to prepare the surface of a specimen for examination via scanning electron microscopy. Suggestions were made for minimizing the possibility of creating such artifacts and for obtaining data for which the relationships between (1) bulk structural features and (2) defects related to aging and breakdown can be more reliably interpreted. Several corroborative experiments were also recommended to supplement the morphology studies.

*601,279*
**PB87-108148** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Hydrolysis of Cross-Linked Polyester Polyurethanes.**
Final rept.,
D. W. Brown, R. E. Lowry, and L. E. Smith. 1984, 7p
Pub. in Polymer Material Science and Engineering 51, p155-161 1984.

Keywords: *Polyurethane resins, *Polyester resins, *Hydrolysis, Crosslinking, Polymers, Films, Degradation, Reprints.

Cross-linked polyester polyurethane films were made by reacting toluene diisocyanate with polyester polyurethane at 100 C for 5-7 days. Mol ratios of isocyanate to urethane were 0.14, 0.55, and 1.10. Sol fractions were 0.79, 0, and 0, respectively. These films and the original polymer were aged at various temperatures and relative humidities, RH. Samples were evaluated by measuring tensile strength, elongation, sol fraction, acid content, and the change in the concentration of alcohol groups. Dense cross-linking greatly extended the time before loss of strength and elongation became severe. Aging at 85 C and 100 and 50% RH eventually made all but the most densely cross-linked polymer completely soluble. A second infinite network probably existed in the latter, which was not hydrolyzed. The initial alcohol concentration was less in the more densely cross-linked films. Concentrations of alcohol and acid increased more slowly in these two films. The effect was especially marked at low RH.

*601,280*
**PB87-113684** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
**Guest Editorial.**
Final rept.,
M. G. Broadhurst, F. Micheron, and Y. Wada. 1981, 1p
Pub. in Special Issue on PVDF (Polyvinylidene Fluoride) and Associated Piezoelectric Polymers, p3 Apr 81.

Keywords: *Ferroelectric materials, *Piezoelectric materials, Ferroelectricity, Polymers, Pyroelectricity, Vinylidene resins, *Vinylidene fluoride.

An introduction to a special issue of Ferroelectrics on Polyvinylidene Fluoride and related Piezoelectric polymers is given. The introduction includes a history of the field, an analysis of its progress, and a speculation about its future.

*601,281*
**PB87-118964** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**FT-IR Studies of Molecular Organization in Polyethylene.**
Final rept.,
B. Fanconi, and D. Sarazin. 1984, 2p
Pub. in Polymer Preprints 25, n2 p173-174 1984.

Keywords: *Polyethylene, *Molecular structure, *Spectroscopic analysis, Infrared spectroscopy, Thermoplastic resins, Reprints, Fourier transform spectroscopy.

FT-IR studies of mixtures of perdeutero polyethylene and polyethylene have been carried out on single crystals suspended in cyclohexane. The spectra are compared to those obtained from dried and pressed single crystal mats to reveal substantial spectral changes caused by mechanical deformation of the crystallites. The impact of these spectral changes on the interpretation of the organization of polyethylene molecules in single crystal textured material is discussed. A method of analyzing the FT-IR spectra of mixed crystals that is based on lattice dynamical calculations and the electro-optical parameter approach for IR intensities is presented. The method has been successfully applied to n-alkane mixtures and an improved spectral measure of local concentration of deuterated molecules is derived. The method shows promise for characterizing the local concentrations of deuterated stems in melt-crystallized polyethylene mixtures.

*601,282*
**PB87-122198** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Investigations in Array Sizing - 3. The Center Distance Finding Technique.**
Final rept.,
A. W. Hartman. 1986, 12p
See also PB86-196011.
Pub. in Powder Technology 46, n2-3 p109-120 1986.

Keywords: *Particle size distribution, Dimensional measurement, Arrays, Microscopy, Polystyrene, Optical measurement, Microphotographs, Reprints, *Microspheres.

The feasibility of measuring the size distribution of microspheres by optical microscopy is investigated for monosize 3 micrometers and 10 micrometers polystyrene material. A new technique for doing this is presented, based on the light-focusing properties of transparent and uniform microspheres that are arranged in a two-dimensional structure of spheres touching each other. When illuminated with parallel light, the spheres bring this light together into small focal spots which are then used as high-resolution markers of sphere position. The sphere center distances are measured with better than 0.5% resolution from scaled microphotographs. The obtained center distance distributions are used to find the diameter distributions of 3.0 micrometers and 10 micrometers polystyrene spheres.

*601,283*
**PB87-122289** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Defect Motion and Relaxation Processes In Polyethylene.**
Final rept.,
D. H. Reneker, and J. Mazur. 1981, 4p
Pub. in International Symposium on Macromolecules, Abstracts of Communications (27th), Strasbourg, France, July 6-9, 1981, v2 p879-882.

Keywords: *Polyethylene, Defects, Relaxation(Mechanics).

The defect in polyethylene known as a point dislocation(1) or twist dispiration loop(2), which transports a chain along its axis through a crystal by a process appropriately called reptation. In the following, the word defect is used not in its general sense but as a short name for a point dislocation. Two sets of experimental data provide quantitative information on the rotation rate of the chain stems around their long axes. One set

is from C-13 nuclear magnetic resonance experiments and the second is from dielectric loss measurements on lightly oxidized polyethylene which contains approximately one polar group per chain stem. Mechanical relaxation data can be interpreted as a consequence of the translation of a defect in a strain field.

*601,284*
**PB87-128146** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Comparative Rates of Heat Release from Five Different Types of Test Apparatuses.**
Final rept.,
V. Babrauskas. 1986, 12p
Pub. in Jnl. of Fire Sciences 4, p148-159 Mar/Apr 86.

Keywords: *Test equipment, *Calorific value, Evaluation, Fire resistant materials, Construction materials, Fire tests, Ignition, Composite materials, Laminated plastics, Flashover, Aircraft cabins, Reprints.

Previously reported rates of heat release using five different bench-scale test methods are compared with each other and against a limited series of large-scale tests. The materials tested were low-flammability wall lining materials, of a construction similar as might be used for aircraft cabin walls. Based on the peak values at different irradiances, three of the methods gave similar results: the Cone Calorimeter, the FMRC Flammability Apparatus, and the Flame Height Apparatus. The other data, from the OSU calorimeter in the thermopile mode and the OSU calorimeter in the oxygen-consumption mode, gave results typically 1/2 of the first three methods. Simple techniques for predicting full-scale performance from bench-scale data are emerging. The preliminary application of these appears promising.

*601,285*
**PB87-134813** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div.
**Up and Down Test Method - E-11 Members Respond.**
Final rept.,
E. H. Jebe, and M. G. Natrella. 1985, 2p
Pub. in ASTM Standardization News 13, n2 p40-41 1985.

Keywords: *Impact tests, *Plastic pipes, Structural plastics, Pipes(Tubes), Reprints, *Up and down method.

The brief note gives a summary of some characteristics of the Up-and-Down Test Method. It is a response by members of ASTM Committee E-11 to an article (previously published in ASTM Standardization News) that stressed some disadvantages of the Method as it was applied to the impact testing of plastic pipe.

*601,286*
**PB87-136651** PC **A08**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Prediction of the Long Term Stability of Polyester-Based Recording Media,**
L. E. Smith, D. W. Brown, and R. E. Lowry. Oct 86, 153p NBSIR-86/3474
See also PB85-160133.

Keywords: *Aging tests(Materials), *Polymeric films, *Magnetic tapes, *Adhesives, *Binders(Materials), Humidity, Storage, Archives, Infrared spectroscopy, Polyethylene terephthalate, Hydrolysis, Stability.

Magnetic data tapes have been aged at several temperatures and relative humidities. Data previously recorded on the tapes was read back after aging and the inability to read such data was used to make a preliminary estimate of tape lifetime. Based on the criterion the authors estimate a useful tape lifetime of 20 years at ambient conditions. The tape lifetime estimate should be considerably more certain by the time of the final report in the series which will be issued in November 1987. There are documented reports of tape failure after ten years of storage under normal room temperature and humidity. Reading failures with rapidly-aged tapes appear to be caused primarily by exudation of material from the binder layer. In order to test the condition of tapes before failure, three tests were devised that measure adhesion or extensibility of the binder layer. Water content and weight changes on aging were also measured. None of these five secondary quantities correlated quantitatively with the ability of a tape transport to read data previously written on the tapes, but some of them are useful indicators of risk.

## Refractory Metals & Alloys

*601,287*
**PB86-213030** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Nicrosil Versus Nisil Thermocouple: The Influence of Magnesium on the Thermoelectric Stability and Oxidation Resistance of the Alloys.**
Final rept.,
N. A. Burley, J. L. Cocking, G. W. Burns, and M. G. Scroger. 1982, 17p
Pub. in Temperature: Its Measurement and Control in Science and Industry, v5 pt2 p1129-1145 1982.

Keywords: *Thermocouples, *Heat resistance alloys, Thermoelectric properties, Nickel alloys, Silicon, Chromium, Magnesium, Oxidation resistance, Reprints.

The new nickel-base alloy thermocouple nicrosil (Ni-14.2 wt.%Cr-1.4 wt.%Si) versus nisil (Ni-4.4 wt.% Si-0.1 wt.%Mg) shows greatly enhanced thermoelectric stability relative to the ANSI standard base-metal thermocouples type E, J, K and T. This is primarily because the component solute levels of chromium and silicon in nicrosil and nisil are high enough to produce greatly enhanced oxidation resistance. The paper reports the effects of additions to the nominal compositions of up to 0.1 wt. % Mg upon the mechanisms of oxidation in air and upon the thermoelectric stability of both nicrosil and nisil at 1100 and 1200 C. The thermoelectric stability and oxidation resistance of nicrosil and nisil were found to be markedly superior to those of type KP and type KN thermoalloys tested lor comparison under the same conditions.

*601,288*
**PB87-104238** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Thermodynamic Properties of bcc Metals.**
Final rept.,
R. A. MacDonald, R. C. Shukla, and D. K. Kahaner. 1985, 6p
Pub. in High Temperatures-High Pressures 17, p665-670 1985.

Keywords: *Transition metals, *Thermodynamic properties, Specific heat, Free energy, Niobium, Tungsten, Reprints.

Lowest-order anharmonic perturbation theory has been used for calculating the Helmholtz free energy for a second-neighbour central-force model of a bee crystal in the high-temperature limit (T > the Debye temperature). The atomic interactions are represented by a modified Morse potential. The equilibrium lattice spacing, and thence the thermal expansion, are obtained. Results for the transition metals Nb and W are presented. Of the other thermodynamic properties, bulk moduli have been found to be very sensitive to the method used to treat the electrons. For the alkali metals, reasonable results were obtained when electron correlation was taken into account. A corresponding calculation for the transition metals is in progress. The results obtained for the thermal expansion and for the lattice contribution to the specific heat at constant volume are presented. The limitations of this model when electrons play a major role in stabilizing the crystal structure are discussed.

*601,289*
**PB87-113585** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Niobium (Columbium)-Platinum Constitution Diagram.**
Final rept.,
R. M. Waterstrat, and B. C. Giessen. 1985, 7p
Grant PHS-DE-02455, Contract SD-90
See also PB80-194392. Sponsored by National Inst. of Dental Research, Bethesda, MD., and Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Metallurgical Transactions A 16A, p1943-1949 Nov 85.

Keywords: *Niobium alloys, *Platinum alloys, Phase diagrams, Intermetallic compounds, Solubility, Phase transformations, X-ray analysis, Reprints.

The Nb-Pt system was investigated over the entire composition range by metallography and X-ray diffraction analysis. The solubility limits of terminal and intermediate phases and solidus temperatures were determined. The presence of six intermediate phases was confirmed. Eight three-phase reactions are described, the mean atomic volumes are given, and crystal chemical relationships among the six homologous T(sub 5)-T(sub 10) systems (T(sub 5) = V, Nb, Ta; T(sub 6) = Pd, Pt) are discussed.

## Wood & Paper Products

*601,290*
**PB87-118147** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**New Approach to the Measurement of Pulp Consistency.**
Final rept.,
A. K. Gaigalas. Jul 86, 1p
Contract DE-AI01-76PRO6010
Sponsored by Department of Energy, Washington, DC.
Pub. in Tappi Jnl. 69, n7 Jul 86.

Keywords: *Papers, *Pulps, Consistency, Dielectric properties, Wavelengths, Pipe flow, Gravimeters, Radio waves, Reprints, *Dielectric constants.

The effective dielectric constant of paper pulp flowing in a pipe with diameter equal to 6.25 inches was determined by measuring the wavelength, frequency, and attenuation of radio waves propagating inside the pipe. The solids percent was obtained from the effective dielectric constant by using a simple mixing model. Good agreement was obtained with values of percent solid obtained from grab sample measurement.

*601,291*
**PB87-131819** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Prediction of the Heat Release Rate of Wood.**
Final rept.,
W. J. Parker. 1986, 10p
Sponsored by Federal Emergency Management Agency, Washington, DC.
Pub. in Proceedings of International Symposium on Fire Safety Science (1st), Gaithersburg, MD., October 7-11, 1985, p207-216 1986.

Keywords: *Wood, *Heat of combustion, Thermal conductivity, Pyrolysis, Thickness, Mathematical models, Moisture, Heat flux, Particle boards, Reprints, Douglas fir.

A method for predicting the heat release rate of wood for different thicknesses, moisture contents, and exposure conditions is described. A model has been set up and calculations have been made on a microcomputer. Heat release rates and effective heats of combustion were measured as a function of time and external radiant flux on 12.5 mm thick dry vertical specimens of Douglas fir particle board. The calculated and measured curves are similar in shape and amplitude but differ significantly in time scale. The initial results with the model are promising.

## General

*601,292*
**PB86-196011** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Investigations in Array Sizing - 2. The Kubitschek Effect.**
Final rept.,
A. W. Hartman. 1985, 4p
See also PB85-151637.
Pub. in Powder Technology 42, n3 p269-272 Jun 85.

Keywords: *Particle size, *Dimensional measurement, Optical measurement, Spheres, Reprints, *Microspheres, Kubitschek effect.

The Kubitschek array correction is detected and measured in microsphere material for the first time. Introduction of two new techniques permitted carrying out the needed dimensional measurements at the 0.01 micrometer level using optical microscopy.

# MATHEMATICAL SCIENCES

## Analysis

*601,293*

**AD-A101 792/0** Not available NTIS
National Bureau of Standards, Washington, DC.
**Extended-Range Arithmetic and Normalized Legendre Polynomials,**
J. M. Smith, F. W. J. Olver, and D. W. Lozier. Mar 77, 14p ARO-14044.8-M
Grants DAAG29-77-G-0003, NSF-GP-32841
Pub. in ACM Transactions on Mathematical Software, v7 n1 p93-95 Mar 81 (No copies furnished by DTIC/NTIS).

Keywords: *Polynomials, *Arithmetic, Algorithms, Exponential functions, Floating point operation, Reprints, Legendre polynomials, Extended range arithmetic, NTISDODXR.

No abstract available.

*601,294*

**AD-A131 521/7** Not available NTIS
National Bureau of Standards, Washington, DC.
**Error Analysis of Complex Arithmetic,**
F. W. J. Olver. 1983, 15p ARO-16928.3-MA
Contract DAAG29-80-C-0032
Availability: Pub. in Computational Aspects of Complex Analysis, p279-292 1983 (No copies furnished by DTIC/NTIS).

Keywords: *Functions(Mathematics), *Error analysis, Algorithms, Precision, Computations, Floating point operation, Reprints.

The lecture begins with a brief account of recent work on unrestricted algorithms or computing mathematical functions, especially the development of error analysis based on a nontraditional definition of relative error. The main part of the talk describes the application of this analysis to real and complex arithmetic and concludes with some new extensions that have been made in complex arithmetic.

*601,295*

**PB86-195625** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
**Asymptotic Behavior of Scaled Singular Value and QR Decompositions.**
Final rept.,
G. W. Stewart. 1984, 7p
Pub. in Mathematics of Computation 43, n168 p483-489 1984.

Keywords: Asymptotic series, Least squares method, Approximation, Reprints, *Matrices, Singular value decomposition, Factorization.

Asymptotic expressions are derived for the singular value decomposition of a matrix, some of whose columns approach zero. Expressions are also derived for the QR factorization of a matrix, some of whose rows approach zero. The expressions give insight into the method of weights for approximating the solutions of constrained least squares problems.

*601,296*

**PB86-214681** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
**Addition of Points to Gauss-Laguerre Quadrature Formulas.**
Final rept.,
D. K. Kahaner, J. Waldvogel, and L. W. Fullerton. Mar 84, 14p
Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. of Scientific and Statistical Computing 5, n1 p42-55 Mar 84.

Keywords: *Gaussian quadrature, Numerical quadrature, Numerical integration, Error analysis, Reprints.

The Gauss-Laguerre quadrature formula is defined by If = the integral from 0 to infinity, of ((e sup -x)f(x)dx) approx. = Summation from (i-1) to n, of ((a sub i, sup (n)) f (zeta sub i, sup (n))), where the numbers a sub i, sup (n) and zeta sub i, sup (n) are weights and nodes. A common method of estimating the error of the rule is to evaluate the quadrature rule for two different values of n and to then compare the difference in the answers. Unfortunately, none of the nodes or weights are in common for the two different quadrature rules, and so the function must be evaluated at each separate node. The authors investigate in the paper the addition of points to the Gauss-Laguerre rule such that the new points are real, lie in the interval of integration, and the associated weights are positive. Such rules enable one to estimate economically the error of quadrature, because the function values at the Gauss-Laguerre abscissae are reused. A collection of suitable low-order formulae are given.

*601,297*

**PB86-215175** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
**Evaluation of L sub 1 Codes Using Polynomial Approximation Problems,**
P. D. Domich, K. L. Hoffman, R. H. F. Jackson, P. B. Saunders, and D. R. Shier. Jun 86, 48p NBSIR-86/3390

Keywords: *Approximation, *Polynomials, Mathematical programming, Nonlinear systems, Computation, Algorithms, Computer applications, UNIVAC - 1108 computers.

The paper presents the methodology and results of a computational experiment which compares the performance of four computer codes which determine the best discrete L sub 1 approximation to a continuous nonlinear function. The experiment uses 320 test problems created by a test problem generator. Several performance measures describe solution quality as well as computational effort.

*601,298*

**PB86-215183** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
**Near-Optimal Starting Solution for Polynomial Approximation of a Continuous Function in the L sub 1 Norm,**
P. D. Domich. Jun 86, 28p NBSIR-86/3389

Keywords: *Approximation, *Polynomials, Computation, Chebyshev functions.

The paper presents a method of selecting a near-optimal starting basis for a large class of polynomial approximation problems in the L sub 1 norm. While it is possible to prove the optimality of these advanced starting solutions for only a small class of problems, empirical evidence indicates the starting bases are nearly optimal for a much larger class of problems. The paper presents the method used to determine the starting basis and a heuristic justification backed by empirical results supporting its use.

*601,299*

**PB86-229689** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**L (sup infinity symbol) Error Bounds In Partial Deconvolution of the Inverse Gaussian Pulse.**
Final rept.,
A. S. Carasso, and N. N. Hsu. Dec 85, 10p
Sponsored by Army Research Office, Research Triangle Park, NC.
Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. of Applied Mathematics 45, n6 p1029-1038 Dec 85.

Keywords: Signal processing, Delta functions, Greens function, Linear systems, Approximation, Reprints, *Impulse response, Time invariant systems, Deconvolution.

When a C(sup infinity symbol) approximation to the Dirac delta-function, in the form of an inverse Gaussian pulse, is used as input into a linear time invariant system, the output waveform is an approximation to that system's Green's function, in which the singularities have been smoothed out. The ill-posed deconvolution problem for the output signal aims at reconstructing these singularities. By exploiting the smoothing properties of the inverse Gaussian kernel, the authors prove that partial deconvolution of the output waveform, given L(sup 2) a priori bounds on the data noise and the unknown Green's function, results in L(sup infinity symbol) error bounds for the regularized solution and its derivatives. Consequently, when the L2 norm of the output noise is sufficiently small, partial deconvolution is a pointwise reliable C(sup infinity symbol) function, which in turn approximates the desired Green's function in many applications.

*601,300*

**PB87-128120** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Some Results on Generalized Elliptic-Type Integrals.**
Final rept.,
S. L. Kalla, S. Conde, and J. H. Hubbell. 1986, 15p
Pub. in Applicable Analysis 22, p273-287 1986.

Keywords: *Elliptic functions, Hypergeometric functions, Asymptotic series, Reprints, Numerical solution.

In the present paper, the authors study a family of integrals for which special cases occur in radiation field problems. They obtain a series expansion and establish its relationship with Gauss' hypergeometric function. Asymptotic expansions valid in a neighborhood, and some recurrence relations are given. Results obtained earlier by Epstein and Hubbell, Weiss, and Kalla follow as particular cases of the formulae established here. Some numerical values are computed.

*601,301*

**PB87-140596** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
**B2DE - A Program for Solving Systems of Partial Differential Equations in Two Dimensions,**
J. L. Blue. Jun 86, 63p NBSIR-86/3411

Keywords: *Elliptic differential equations, *Partial differential equations, *Nonlinear differential equations, *Computer programs, B2DE computer program, Two-dimensional calculations, Laplace equation, Interactive graphics, Fortran 77 programming language.

B2DE is a program for solving systems of nonlinear elliptic partial differential equations (PDEs) in two dimensions. The program is a collection of modules with an interactive driver. Many types of interactive graphics plots are included. Users may modify the driver, and may be able to construct a 'black box' program for a restricted class of PDEs. B2DE is available from the author.

## Operations Research

*601,302*

**PB86-210069** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
**Projections onto Order Simplexes.**
Final rept.,
S. J. Grotzinger, and C. Witzgall. 1984, 24p
Pub. in Applied Mathematics and Optimization 12, n3 p247-270 1984.

Keywords: Quadratic programming, Curve fitting, Reprints, *Isotone regression, Isotone regression, Kuhn-Tucker theory.

Isotone regression techniques are reinterpreted and extended to include upper and lower bounds on the ordered sequences in question. This amounts to solving the shortest distance problem for the order simplex in (S sup n) in (R sup n). An O(n) algorithm is presented for this problem, verified via the Kuhn-Tucker conditions, and explained geometrically in terms of the Lagrange multipliers. In the context, isotone regression techniques are interpreted in terms of orthogonal projections onto faces of the order simplex (S sup n).

These projections provide a succinct characterization of the descent directions required for the design of gradient projection methods for minimizing differentiable functions on (S sup n).The latter problem arises in parameterized curve fitting. The authors conclude by considering generalizations of these techniques.

*601,303*
**PB87-104436** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
**Polyadic Third-Order Lagrangian Tensor Structure and Second-Order Sensitivity Analysis with Factorable Functions,**
R. H. F. Jackson, and G. P. McCormick. Aug 85, 68p NBSIR-85/3222
Prepared in cooperation with George Washington Univ., Washington, DC. Dept. of Operations Research.

Keywords: *Nonlinear programming, Perturbation theory, Tensors, Theorems, Constrained optimization, Sensitivity analysis, Matrices.

Second-order sensitivity analysis methods are developed for analyzing the behavior of a local solution to a constrained nonlinear optimization problem when the problem functions are perturbed slightly. Specifically, formulas involving third-order tensors are given to compute second derivatives of components of the local solution with respect to the problem parameters. When in addition, the problem functions are factorable, it is shown that the resulting tensors are polyadic in nature.

## Statistical Analysis

*601,304*
**AD-A142 580/0** PC **A02**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Errors-in-Variables for Binary Regression Models,**
R. J. Carroll, C. H. Spiegelman, K. K. G. Lan, K. T. Bailey, and R. D. Abbott. 1984, 8p AFOSR-TR-84-0519
Contract F49620-82-C-0009
Pub. in Biometrika, v71 n1 p19-25 1984.

Keywords: *Mathematical models, Binary arithmetic, *Regression analysis, Errors, *Cardiovascular diseases, Variables, Mathematical prediction, Measurement, Estimates, Probability, Coronary disease, Risk, Blood pressure, Cholesterol, Reprints, Logistic regression, Probit regression.

The authors consider in detail probit and logistic regression models when some of the predictors are measured with error. For normal measurement errors, the functional and structural maximum likelihood estimates (MLE) are considered; in the functional case the MLE is not generally consistent. Non-normality in the structural case is also considered. By an example and a simulation, the authors show that if the measurement error is large, the usual estimate of the probability of the event in question can be substantially in error, especially for high risk groups.

# MEDICINE & BIOLOGY

## Biochemistry

*601,305*
**PB86-185493** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Active Site of RNase: Neutron Diffraction Study of a Complex with Uridine Vanadate, a Transition-State Analog.**
Final rept.,
A. Wlodawer, M. Miller, and L. Sjolin. 1983, 4p
Pub. in Proceedings of the National Academy of Sciences 80, n12 p3628-3631 1983.

Keywords: *Ribonuclease, Enzymes, Catalysis, Neutron diffraction, X ray diffraction, Hydrogen bonds.

A complex of PNase A with a transition state analog, uridine vanadate, has been studied by a combination of neutron and X-ray diffraction. The vanadium atom occupies the center of a distorted trigonal bipyramid, with the ribose oxygen O2' at the apical position. Contrary to expectations based on the straightforward interpretation of the known in-line mechanism of action of RNase, NE2 of His 12 was found to form a hydrogen bond to the equatorial oxygen O8, while NZ of Lys 41 makes a clear hydrogen bond to the apical O2'. Nitrogen NDI of His 119 appears to be within a hydrogen bond distance of the other apical oxygen, O7. Two other hydrogen bonds between the vanadate and the protein are made by NE2 of Gln 11 and by the amide nitrogen of Phe 120. The observed geometry of the complex may necessitate reinterpretation of the mechanism of action of RNase.

*601,306*
**PB86-189123** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
**Iron Electronic Structure in Oxyhemoglobin and Carboxypeptidase Digested Derivatives.**
Final rept.,
B. Balko, E. Bucci, R. L. Berger, L. J. Swartzendruber, and J. X. Montemarano. 1984, 10p
Pub. in Jnl. of Biochemical and Biophysical Methods 10, n1-2 p55-64 1984.

Keywords: *Hemoglobin, *Iron, *Magnetic fields, Reprints, *Electronic structure, Mossbauer effect.

Mossbauer experiments were performed on the oxy-derivatives of human hemoglobin and its products of digestion with carboxypeptidases. The hemoglobins were chemically enriched to 95% in 57Fe, and were free from hemochrome impurities. Spectra were taken at low temperatures in the presence and absence of a 5.0 T magnetic field. It was observed that the enzymatic digestions which remove residues at least 16 angstroms from the iron of the nearest heme appear to modify the electronic environment of the metal.

*601,307*
**PB86-210028** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Separation of Peptides by High-Performance Ion-Exchange Chromatography.**
Final rept.,
M. Dizdaroglu. 1984, 21p
Pub. in CRC Handbook HPLC Separation of Amino Acids, Peptides, Proteins, v2 p23-43 1984.

Keywords: pH effect, Polymers, Silicia, Temperature, Reprints, *Ion exchange chromatography, *Peptide separations.

The use of high-performance ion-exchange chromatography in peptide separations has been reviewed. Separation profiles of peptides from various sources on silica-based or polymeric ion-exchangers are presented. A recently developed method using a weak anion-exchanger is discussed in detail.

*601,308*
**PB86-229424** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Formation of Cytosine Glycol and 5,6-Dihydroxycytosine in Deoxyribonucleic Acid on Treatment with Osmium Tetroxide.**
Final rept.,
M. Dizdaroglu, E. Holwitt, M. P. Hagan, and W. F. Blakely. 1986, 6p
Sponsored by Armed Forces Radiobiology Research Inst., Bethesda, MD.
Pub. in Biochemical Jnl. 235, p531-536 1986.

Keywords: *Deoxyribonucleic acids, Gas chromatography, Mass spectroscopy, Reprints, *Repair enzymes, *Glycol/cytosine, *Cytosine/dihydroxy, *Oxide/osmium-tetra.

OsO4 selectively forms thymine glycol lesions in DNA. In the past, OsO4-treated DNA has been used as a substrate in studies of DNA repair utilizing base-excision repair enzymes such as DNA glycosylases. Using a methodology developed recently for characterization of oxidative base damage in DNA, the authors provide evidence for the formation of cytosine glycol and 5,6-dihydroxycytosine moieties, in addition to thymine glycol, in DNA on treatment with OsO4. The implications of these findings relative to studies of DNA repair are discussed.

*601,309*
**PB86-239746** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**Binding of Pt(NH3)3 (2+) to Nucleic Acid Bases.**
Final rept.,
H. Basch, M. Krauss, W. J. Stevens, and D. Cohen. 1986, 5p
Pub. in Inorganic Chemistry 25, n5 p684-688 1986.

Keywords: *Chemical bonds, *Deoxyribonucleic acids, Nucleic acids, Ligands, Reprints, *Platinum amine complex, Binding energy, Nucleotides, Effective potential.

The bonding of Pt-amine complexes to DNA is modeled by calculating the SCF binding energy of Pt(NH3)3(2+) to gaunine, adenine, cytosine, and thymine. A relativistic effective potential is used to represent the core electrons of Pt and compact effective potentials were also used to replace the core electrons in carbon, nitrogen, and oxygen to simplify the calculation of these large molecules. In order to analyze the bonding, SCF calculations were also done for H2O, NH3, imidazole, pyrimidine, and 2- and 4-pyrimidone. The binding is calculated to have a large electrostatic contribution but there is a significant contribution from polarization of the base. The valence all-electron energy can be reproduced by an SCF energy for a system where the Pt(NH3)3(2+) complex is replaced by an effective charge, (Z sub eff). The binding order for all the sites on the nucleic acid bases was calculated by the means.

*601,310*
**PB87-100236**
(Order as PB87-100186, PC **A08**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Inorganic Materials Biotechnology: A New Industrial Measurement Challenge,**
G. J. Olson, and F. E. Brinckman. Jun 86, 9p
Sponsored by Office of Naval Research, Arlington, VA.
Included in Jnl. of Research of the National Bureau of Standards, v91 n3 p139-147 May-Jun 86.

Keywords: *Metals, *Metalloids, Microorganisms, Materials recovery, Organometallic compounds, Inorganic compounds, *Microbial processes, *Biotechnology, Heavy metals, Metabolites.

Biotechnological processing of inorganic, heavy elements has only begun to emerge as the authors start to understand microbial strategies and mechanisms of heavy element transformation. Chemical speciation of key, diagnostic intermediates and products of bioprocessing in gas liquid, and cellular phases, and on surfaces, is required to understand and optimize important reactions. Recent discoveries of microorganisms in metal-enriched thermal environments, and further investigations into production of exocellular metal transforming metabolites, offer exciting prospects for development of new technologies for strategic and precious materials recovery and processing.

*601,311*
**PB87-106084** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Weak Anion-Exchange High-Performance Liquid Chromatography of Peptides.**
Final rept.,
M. Dizdaroglu. 1985, 21p
Pub. in Jnl. of Chromatography 334, n1 p49-69 1985.

Keywords: *Peptides, *Chromatographic analysis, Chemical analysis, Anion exchanging, Reprints, Liquid chromatography.

In the survey, the principles and applications of a method recently developed for peptide separations are given. This method uses a bonded weak anion-exchange column and mixtures of volatile triethylammonium acetate buffer and acetonitrile as eluent. Its applications to the separation of a large number of peptides including diastreomeric and other closely related peptides are discussed. Separation of the enzymatic digests of some proteins is also presented. The complementary use of this method to the reversed-phase methods is outlined and their combined use for separation of enzymatic digests of proteins and assessment of purity of synthesized peptides is demonstrated. The results reviewed show that the weak anion-exchange method is an excellent approach for peptide

separations and could be an important partner of reversed-phase methods for achieving optimal results.

*601,312*
**PB87-106092** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Separation of Sequence Isomeric Dipeptides by High-Resolution Gas Chromatography.**
Final rept.,
M. Dizdaroglu. 1985, 5p
Pub. in Jnl. of Chromatography 318, n2 p384-388 1985.

Keywords: *Chromatographic analysis, *Peptides, Gas chromatography, Reprints, Peptide sequencing.

Trimethylsilyl derivatives of some sequence isomeric dipeptides were separated by high-resolution gas chromatography on a fused silica capillary column. The nominal structures of the separated isomers were confirmed by gas chromatography-mass spectrometry. The relevance of this work to sequencing of polypeptides by using dipeptidyl peptidases and gas chromatography-mass spectrometry is discussed.

*601,313*
**PB87-106696** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Characterization of Free Radical-Induced Base Damage in DNA at Biologically Relevant Levels.**
Final rept.,
M. Dizdaroglu, and D. S. Bergtold. 1986, 5p
Sponsored by Armed Forces Radiobiology Research Inst., Bethesda, MD.
Pub. in Analytical Biochemistry 156, p182-188 1986.

Keywords: *Deoxyribonucleic acid, *Free radicals, Chemical radicals, Chromatographic analysis, Reprints, *Biological radiation effects, DNA damage, DNA repair, Hydroxyl radicals, Carcinogenesis.

DNA damage induced by oxygen radicals, e.g., hydroxyl radicals generated in living cells either by cellular metabolism or external agents such as ionizing radiations, appears to play an important role in mutagenesis, carcinogenesis, and aging. Elucidation of the chemical nature of such DNA lesions at biologically significant quantities is required for the assessment of their biological consequences and repair. For this purpose, a sensitive method using gas chromatography-mass spectrometry with the selected-ion-monitoring technique (GC-MS/SIM) was developed in the present work. DNA was exposed to hydroxyl radicals and hydrogen atoms produced by ionizing radiation in N2O-saturated aqueous solution. This technique permitted the detection and characterization of a large number of free radical-induced based products of DNA. Because the GC-MS/SIM technique provides rapid and absolute characterization of a large number of free radical-induced base products simultaneously and does so with a high degree of sensitivity, it is suggested as an ideal analytical tool for the identification of such base lesions in cellular DNA, for their detection in biological fluids, and for the study of their repair and biological consequences.

*601,314*
**PB87-117966** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Free-Radical-Induced Formation of an 8,5' - Cyclo-2' - Deoxyguanosine Molety in Deoxyribonucleic Acid.**
Final rept.,
M. Dizdaroglu. 1986, 8p
Pub. in Biochemical Jnl. 238, p247-254 1986.

Keywords: Free radicals, Deoxyribonucleic acids, Chemical analysis, Gas chromatography, Mass spectroscopy, Reprints, *Cyclodeoxyguanosine, *Guanosine/deoxy, *DNA, Gamma radiation, Enzymatic hydrolysis.

Isolation and identification of a novel OH-induced product, namely an 8,5'-cyclo-2'-deoxyguanosine moiety, in DNA and 2'-deoxyguanosine are described. OH radicals were generated in dilute aqueous solutions by gamma-irradiation. Analyses of 2'-deoxyguanosine and enzymic hydrolysates of DNA by gas chromatography-mass spectrometry (g.c.-m.s.) after trimethylsilylation showed the presence of 8,5-cyclo-2'-deoxyguanosine on the basis of its fragment ions. The use of g.c.-m.s. with the selected-ion monitoring technique facilitated the detection of 8,5'-cyclo-2'-deoxyguanosine in DNA at radiation doses as low as 1 Gy. Its mechanism of formation probably involves hydrogen atom abstraction by OH radicals from the C-5' of the 2'-deoxyguanosine moiety followed by intramolecular cyclization with the formation of a covalent bond between the C-5' and C-8 and subsequent oxidation of the resulting N-7-centred radical.

*601,315*
**PB87-118600** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Mathematical Models for Ligand-Receptor Binding: Real Sites, Ghost Sites.**
Final rept.,
I. M. Klotz, and D. L. Hunston. 1984, 3p
Pub. in Jnl. of Biological Chemistry 259, n16 p60-62 1984.

Keywords: *Ligands, Binding, Enzymes, Reaction kinetics, Mathematical models, Molecular structure, Reprints, *Asparate transcarbamylase.

In the basic life sciences the term 'model' implies a physical, chemical or molecular construct that provides a representation for the interpretation of experimental observations. To the mathematical statistician, however, a 'model' is a mathematical expression for correlating data, which may or may not have roots in a molecular picture. With regard to ligand-receptor interactions, the mathematical model used plays a crucial role in extrapolations of binding measurements. Regardless of the statistical goodness of fit of the data to an equation, the relationships of the parameters of a mathematical formalism to the molecular features of ligand-receptor complexes is generally very complex. Oversimplified interpretations of the molecular significances of the constants derived from binding measurements are unwarranted, unless one has independent information from molecular probes.

*601,316*
**PB87-118691** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Molecular Dynamics Simulation Study of a Two-Dimensional Fluid Mixture System: A Model for Biological Membranes.**
Final rept.,
R. D. Mountain, R. M. Mazo, and J. J. Volwerk. 1986, 11p
Grants PHS-GM-25698, NSF-CHE82-14688
Sponsored by Public Health Service, Rockville, MD., and National Science Foundation, Washington, DC.
Pub. in Chemistry and Physics of Lipids 40, p35-45 1986.

Keywords: *Lipids, Membranes, Computerized simulation, Reprints, *Protein lipid ordering, Molecular dynamics.

The computer simulation technique of molecular dynamics was applied to a model two-dimensional fluid mixture system to examine the short-range ordering of lipid and protein molecules in biological membranes. The model system consists of small disks (lipids) and large disks (proteins) with a radius ratio of 6, constrained to move in a plane. The particles interact with pairwise additive repulsive short range potentials, so as to simulate hard disks. Periodic boundary conditions are assumed in order to minimize boundary effects. For values of the number density of the small disks and of the temperature appropriate for a lipid membrane, the fraction, f, if small disks 'next to' at least one large disk was computed by molecular dynamics. This was done as a function of concentration and for several definitions of 'next to'. The molecular dynamics results show that, at moderately low mole fractions of the large disks, the calculated values of f deviate noticeably from the linear relation which would be expected in the absence of protein-protein proximity effects. The results are discussed in terms of current models of lipid-protein ordering in biological membranes.

*601,317*
**PB87-120218** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
**Oxidation of Ascorbate and a Tocopherol Analogue by the Sulfite Derived Radicals SO3(1-) and SO5(1-).**
Final rept.,
R. E. Huie, and P. Neta. 1985, 6p
Pub. in Chem.-Biol. Interact. 63, n1-2 p233-238 1985.

Keywords: *Free radicals, *Oxidation, *Sulfites, Chemical reactions, Chemical radicals, Tocopherol, Reprints, *Ascorbate, *Chemical reaction kinetics, Peroxysulfite radicals, Sulfite radicals.

The sulfite radical, SO3(1-), was produced by the pulse radiolytic oxidation of sulfite or bisulfite and its reactions followed by kinetic spectrophotometry. It was found to be a mild oxidant, reacting with ascorbate with k = 9.2 x 10 to the 6th power/Ms at pH = 6.8 and with trolox (a water-soluable tocopheral analogue) with k approx. 1 x 10 to the 6th power/Ms at pH = 9. It also reacts rapidly with O2 (k = 1.5 x 10 to the 9th power/Ms) to form the peroxysulfite radical SO5(1-), which reacts with ascorbate with k = 1.4 x 10 to the 8th power/Ms at pH = 6.8 and with trolox with k = 1.2 x 10 to the 7th power/Ms at pH = 9.

*601,318*
**PB87-127973** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Thermodynamics of Carbohydrate Isomerization Reactions: The Conversion of Aqueous Allose to Psicose.**
Final rept.,
Y. B. Tewari, and R. N. Goldberg. 1986, 4p
Pub. in Biophysical Chemistry 24, p291-294 1986.

Keywords: *Carbohydrates, Thermodynamics, Chemical reactions, Chromatographic analysis, Hexoses, Pentoses, Enthalpy, Reprints, *Psicose, *Allose.

The thermodynamics of the conversion of aqueous d-psicose to d-allose has been investigated using high-pressure liquid chromatography. The reaction was carried out in phosphate buffer at pH 7.4 over the temperature range 317.25-349.25 K. The following results are obtained for the conversion process at 298.15 K: delta G = -1.41 + or - 0.09 kJ/mol, delta H = 7.42 + or - 1.7 kJ/mol, and delta C (sub p) = 67 + or - 50 J/mol K. An approximate equilibrium constant of 0.30 is obtained at 333.15 K for the conversion of aqueous D-psicose to D-altrose. Available thermodynamic data for isomerization reactions involving aldohexoses and aldopentoses are summarized.

*601,319*
**PB87-132072** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Thermodynamics of the Hydrolysis of Adenosine 5'-triphosphate to Adenosine 5'-diphosphate.**
Final rept.,
E. Gajewski, D. K. Steckler, and R. N. Goldberg. 1986, 5p
Pub. in Jnl. of Biological Chemistry 261, n27 p12733-12737, 25 Sep 86.

Keywords: *Enthalpy, Hydrolysis, Thermodynamic properties, Chemical reactions, Specific heat, Reprints, *ADP, *ATP, Heat capacity.

The enthalpy of hydrolysis of the enzyme-catalyzed (heavy meromyosin) conversion of adenosine 5'-triphosphate (ATP) to adenosine 5'-diphosphate (ADP) and inorganic phosphate has been investigated using heat-conduction microcalorimetry. Enthalpies of reaction were measured as a function of ionic strength (0.05-0.66 mol/kg), pH (6.4-8.8), and temperature (25-37 degC) in Tris/HCl buffer. The measured enthalpies were adjusted for the effects of proton ionization and metal ion binding, protonation and interaction with the Tris buffer, and ionic strength effects to obtain a value of delta H(sup 0) = -20.5 + or - 0.4 kJ/mol at 25 deg C for the process, ATP (4-)(aq) + H2O(l) = ADP(3-)(aq) + HPO 4(2-) (aq) + H(1+) (aq) where aq is aqueous and l is liquid.

*601,320*
**PB87-134698** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Tryptophan Metabolites as Antioxidants.**
Final rept.,
S. V. Jovanovic, and M. G. Simic. 1985, 7p
Pub. in Life Chem. Rep. 3, n1-2 p124-130 1985.

Keywords: *Tryptophan, Amino acids, Free radicals, Reaction kinetics, Reprints, *Antioxidants, Metabolites, Pulse radiolysis.

Hydroxy-indole derivatives, metabolic products of tryptophan, were shown to be a new class of potent endogenous antioxidants. Kinetics and mechanisms of

their reactions with free radicals in general and tryptophan radical in particular are presented.

## Clinical Chemistry

*601,321*

**PB86-242245** (Order as PB86-242179, PC **A04**/MF **A01**)
Veterans Administration Medical Center, Omaha, NE.
**Storage and Pre-Neutron Activation Analysis Treatment for Trace Element Analysis in Urine,**
A. J. Blotcky, and E. P. Rack. 29 Oct 85, 10p
Prepared in cooperation with Nebraska Univ.-Lincoln.
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p93-102 Mar-Apr 86.

Keywords: Storage, *Biomedical sampling, *Trace element analysis, *Neutron activation analysis, *Urinalysis.

The problems regarding storage and pre-neutron activation analysis treatment for the elements aluminum, calcium, vanadium, selenium, copper, iodine, zinc, manganese, and magnesium in a urine matrix are reviewed. The type of collection and storage procedure and pre-neutron activation analysis treatment of urine depend on the specific trace element; that is, its inherent physical and chemical properties. Specifically polyethylene in teflon containers are the most suitable for general determinations. Whether any preservative is added would depend upon the stability of the trace element and its tendency for surface adsorption. Preferably preservatives should contain no radioactivatable elements for maximum efficacy. Freeze drying or packing urine shipments under dry ice needs to be explored on an individual basis. Each pre- or post-neutron activation analysis treatment is specific and optimized for the trace element analyzed.

## Clinical Medicine

*601,322*

**PB86-200714** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Modification of Cements Containing Vanillate or Syringate Esters.**
Final rept.,
G. M. Brauer, J. W. Stansbury, and D. Flowers. 1986, 7p
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Dental Materials 2, p21-27 1986.

Keywords: *Dental materials, Dental supplies, Toxicity, Zinc oxides, Esters, Fluorides, Reprints, *Vanillate/hexyl, *Syringate/ethyl-hexyl.

Addition of small concentrations of acid, metals or fluorides to vanillate or syringate dental cements was studied in order to improve their physical properties and anticariogenic behavior. Incorporation of acids into cement formulations lowers their setting time. Coating a portion of the zinc oxide powder ingredient with propionic acid offers a convenient way of adjusting the cure to a rate most suitable for clinical applications. The resulting cements are non-brittle, have high strength, low solubility and bond strongly to non-precious metals, porcelain or composites. Cements with zinc undecylate are flexible and may be useful as soft tissue packs. Metallic powders do not act as reinforcing agents for these cements. Hexyl vanillate or ethylhexyl vanillate or ethylhexyl syringate cements can be prepared by adding 0.1% to 1% fluoride salts such as NaF, ZrF4, ZnF2 or dimethylaminoethyl methacrylate hydrofluoride to the powder ingredient.

*601,323*

**PB86-209657** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
**Use of NBS (National Bureau of Standards) Standard Reference Materials in Validating Trace Element Determinations in Biological Materials.**
Final rept.,
R. Alvarez. 1985, 3p
Pub. in Proceedings of International Symposium on Trace Elements in Man and Animals (5th), Aberdeen (Scotland), June 29-July 4, 1984, p655-657 1985.

Keywords: Calibration, Metals, Metabolism, Bioassay, *Standard reference materials, *Biological materials, *Trace elements.

Analyses of biological materials for trace elements often disagree seriously. Yet, accurate analyses are indispensable to understand the role of trace elements in metabolic processes. One approach towards obtaining accurate trace element determinations is through the use of Certified Reference Materials such as the Standard Reference Materials issued by NBS. In general, SRM's are homogeneous stable materials with certified chemical or physical properties for use in calibrating instruments, validating laboratory data, developing methods of known accuracy, and referring data from different laboratories to a common base. Whenever possible SRM's are certified on the basis of accuracy rather than method-dependent analyses. Certified concentrations are based either on the results of a definitive method or on the concordant results of two or more independent analytical methods.

*601,324*

**PB86-212065** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.
**Dielectric Phantoms for Electromagnetic Radiation,**
M. G. Broadhurst, C. K. Chiang, and G. T. Davis. Mar 86, 64p NBSIR-86/3355
Sponsored by Food and Drug Administration, Rockville, MD. Center for Devices and Radiological Health.

Keywords: Electromagnetic radiation, Models(Simulation), Design, Performance, Muscles, Dielectric constant, *Health physics, *Phantoms, *Radiation effects.

The report describes the design and performance of a synthetic material that has the same dielectric heating characteristics as living muscle in the 1-1000 MHz frequency range. The dielectric phantom is a combination of four components: (1) a 50/50 solution of ethylene carbonate and propylene carbonate chosen to have the same dielectric constant as water, (2) an organic salt to provide the same conductivity as biological electrolytes, (3) flakes of polyethylene terephthalate to provide the interfacial polarization that occurs at cell walls in biological tissue and (4) an inorganic and a polymeric gelling agents to provide mechanical rigidity. The resulting composite material is more stable to biological attack and drying than are existing aqueous based phantom materials, and its dielectric properties are more closely matched to those of natural tissues over most of the frequency range of interest.

*601,325*

**PB86-231503** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Water on Apatites.**
Final rept.,
D. N. Misra. 1986, 6p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Calcified Tissue International 38, p333-338 1986.

Keywords: *Calcium phosphates, *Water, *Adsorption, Bones, Area, Surfaces, Reprints, Tooth enamel.

Adsorption of water was studied gravimetrically at 23 deg C in an open system at several relative humidities on a variety of apatitic calcium phosphates including enamel, deproteinized enamel and bone mineral. The amount of adsorbed water increases linearly with the surface areas of the synthetic apatites and does not appear very sensitive to calcium to phosphorus ratio of the apatites. The adsorption results correlate very well up to about two monolayers with a conventionally determined isotherm. Higher uptake of water even by 'deproteinized' enamel or bone may be due to the presence of pore structure and imcompletely removed organic matter.

*601,326*

**PB86-241890** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Determination of Serum Creatinine by Isotope Dilution Mass Spectrometry as a Candidate Definitive Method.**
Final rept.,
M. J. Welch, A. Cohen, H. S. Hertz, K. J. Ng, and R. Schaffer. 1986, 5p
Pub. in Analytical Chemistry 58, n8 p1681-1685 Jul 86.

Keywords: *Chemical analysis, Chemical analysis, Mass spectroscopy, Reprints, *Creatinine, Isotope dilution, Standard reference materials, Carbon 13.

An Isotope dilution mass spectrometric (ID/MS) method for serum creatinine is described which uses creatinine-(13)C2 as the labeled internal standard. Creatinine is separated from creatine and converted to the ethyl ester of N-(4,6-dimethyl-2-pyrimidinyl)-N-methylglycine. Combined capiliary column gas chromatography and electron impact mass spectrometry are used to obtain the abundance ratio of the unlabeled and labeled (M-COOC2H5)(H) ions from the derivative. Quantitation is achieved by measurement of each sample between measurements of two standards whose unlabeled/labeled ratios bracket that of the sample. The high precision and absence of significant bias qualify the method as a candidate definitive method.

*601,327*

**PB87-106001** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Theory of Polymer Composites.**
Final rept.,
R. L. Bowen, D. L. Menis, L. E. Setz, and K. A. Jennings. 1985, 13p
Sponsored by National Institutes of Health, Bethesda, MD., and American Dental Association Health Foundation, Chicago, IL.
Pub. in Posterior Composite Resin Dental Restorative Materials, p95-107 1985.

Keywords: *Dental materials, *Glass particle composites, Dentistry, Composite materials, Polymers, Reinforced plastics, Reprints.

Particulate reinforcing glass fillers are used to improve the physical properties of resins used to restore teeth. Certain aluminoborosilicate glass formulations can be phase-separated by appropriate heat treatment inducing a high-silica phase and a low-silica phase with interpenetrating, interconnected morphology of both vitreous phases. Particles of such glass can be acid-etched to produce microporosity in the surface. The depth of these interconnecting surface asperities can be controlled by the amount of strong acid used in the etching process. The amount of acid was found to correlate with the nitrogen B.E.T. (Brunauer, Emmett, Teller) surface area. When perfected, these materials are expected to yield improved dental composite resin restorative formulations having better strength, polishability, and durability under oral conditions.

## Dentistry

*601,328*

**PATENT-4 616 073** Not available NTIS
Department of Health and Human Services, Washington, DC.
**Hydrophobic Dental Composites Based on a Polyfluorinated Dental Resin.**
Patent,
J. M. Antonucci. Filed 9 Aug 84, patented 7 Oct 86, 12p PB87-121232, PAT-APPL-6-639 673
Supersedes PB85-116440.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Patents, *Dental materials, *Composite materials, *Fluorine organic compounds, Polymers, Performance evaluation.

Dental resin systems prepared from polyfunctional or monofunctional highly-fluorinated methacrylate prepolymers are described. Preferred systems comprise (a) a major amount of a polyfluorinated aligomeric polyfunctional methacrylate such as (PFMA), preferably in

combination with a diluent monomer such as 1,10-decamethylene dimethacrylate (DMDMA), methylmethacrylate (MMA), neopentyl dimethacrylate (NPDMA), 1,6-hexamethylene dimethacrylate (HMDMA), etc., or mixtures thereof; and (b) a minor amount of a polyfluorinated monofunctional methacrylate (PFMMA), such as 1,1-dihydropentadecafluorooctyl methacrylate (PDFOMA) as a minor or secondary diluent monomer in a non-hydroxylated bis-GMA resin system.

*601,329*
**PB86-160157** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Base Metal Alloys In Restorative Dentistry.**
Final rept.,
R. W. Hinman, and J. A. Tesk. 1984, 14p
Pub. in Advanced Restorative Dentistry, ch17 p281-294 1984.

Keywords: *Dental materials, *Alloys, *Metals, Reprints.

The use of base (nonprecious) metal alloys in dentistry is presented. Relevant physical and mechanical properties are described. Some pertinent comparisons of differences between gold and base metal alloys are cited. Attention is focused on processing of prosthetic dental devices with emphasis on casting, soldering, and porcelain veneering; these are primary operations requiring special attention.

*601,330*
**PB86-160744** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Environmental Damage and Wear of Dental Composite Restoratives.**
Final rept.,
J. E. McKinney. 1985, 15p
Pub. in Proceedings of the International Symposium on Posterior Composite Resin Dental Restorative Materials, St. Martin, Caribbean, January 16-19, 1985, p331-347.

Keywords: *Dental materials, Corrosion, Polymers, Restoration, Solubility.

Microhardness and pin-disc wear measurements are used to determine in vivo degradation mechanisms for dental composite restorations. In order to simulate in vivo conditions, the wear test specimens are preconditioned in organic food simulating liquids, which have the potential to damage the polymer matrix; and intraoral acids and water, which have the potential to damage the inorganic filler. Subsequent wear and hardness may be influenced considerably by the chemical damage caused by preconditioning. The matrix damage is quantitized by using the solubility parameter as an independent variable. The filler damage is interpreted in terms of static and stress corrosion, the latter of which occurs during wear. Methods are suggested for improving both the matrix and filler to enhance durability of composite restorations by eliminating, or reducing, vulnerability to intraoral environmental attack.

*601,331*
**PB86-160751** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Chemical Softening and Wear of Dental Composites.**
Final rept.,
J. E. McKinney, and W. Wu. Nov 85, 6p
Contract N01-DE-3-0001
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Jnl. of Dental Research 64, n11 p1326-1331 Nov 85.

Keywords: *Dental materials, *Composite materials, *Polymers, *Wear tests, *Softening, Solubility, Surfaces, Degradation, Solvents, Plastics, Reprints.

The purpose of the work was to determine the influence of chemical food-simulating liquids on the wear of various commercial dental composite restoratives. In many cases, pre-conditioning the restoratives in these liquids for one week produced swelling of the polymer matrix and considerable surface damage. The resulting degradation reduced the hardness and enhanced the wear as measured by a pin-and-disc apparatus. Four kinds of commercial composites were investigated: a conventional quartz-filled, a strontium-glass-filled, a visible-light-activated, and a microfilled composite.

*601,332*
**PB86-191327** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Adsorption of Zirconyl Salts and Their Acids on Hydroxyapatite: Use of the Salts as Coupling Agents to Dental Polymer Composites.**
Final rept.,
D. N. Misra. 1985, 4p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of Dental Research 64, n12 p1405-1408 Dec 85.

Keywords: *Preventive dentistry, *Acids, *Dental enamel, Adsorption, Composite materials, Reprints, Hydroxyapatite, Zirconyl salts.

Zirconyl methacrylate (1) and zirconyl-2-ethylhexanoate (II) were synthesized, and their adsorption isotherms from solutions onto synthetic hydroxyapatite were studied. The isotherms of methacrylic and 2-ethylhexanoic acids were also determined from the same solvents. The adsorption of I was irreversible from methylene chloride, and that of II was irreversible from cyclohexane. The adsorption in both cases was constant from solutions above a certain concentration, and exhaustive below the threshold concentration. Both compounds rendered the dried apatite powder extremely hydrophobic; however, the adsorbate was slowly washed off by excess water.

*601,333*
**PB86-193570** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Dental Applications.**
Final rept.,
G. M. Brauer, and J. M. Antonucci. 1986, 22p
Grant Y01-DE-30001
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Encyclopedia of Polymer Science and Engineering 4, p698-719 1986.

Keywords: *Dental materials, Resins, Composite materials, Adhesives, Polymers, Reprints.

Plastics have been edging into the dental market for the last fifty years. The consumption of resins for dental prosthetic devices, restorative, impression materials and sundries amounts to over 500 tons. Methacrylates are the most widely used resins for the construction of dentures, although many other polymers have been evaluated. Predominance of acrylics is not surprising since the monomer-polymer dough can be polymerized readily and has minimal curing shrinkage. The hardened materials are strong, lifelike, have good color and dimensional stability and are biocompatible with the oral tissues. Miscellaneous uses of these resins include tissue conditioners, crown and bridge resins, mouth protectors, splints, impression trays and patterns for metal castings. Over 13 million acrylic teeth are made annually in the U.S. They have a natural appearance, low breakage, bond to resin base and can be polished. Composites based on dimethacrylate have been very successful in non-stress bearing areas as anterior restoratives where esthetics is of prime importance.

*601,334*
**PB86-200698** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**History of the International Association for Dental Research Wilmer Souder Award in Dental Materials with a Short Biography of Wilmer Souder.**
Final rept.,
G. C. Paffenbarger, and N. W. Rupp. 1986, 4p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Dental Materials 2, p49-52 1986.

Keywords: *Certification, *Dental materials, Specification, *Handwriting.

In the 39 years that Dr. Wilmer Souder was associated with the National Bureau of Standards, he accumulated many awards in several disciplines. The principal areas of his recognition, criminology and dental materials research, were founded in his interest in and capability of making precise length measurements. In 1919 the Army Dental Corps asked the Bureau to assist in formulating a specification for the purchase of alloys for dental amalgam. Dr. Souder agreed to take on the assignment. From that beginning the Dental Materials Section grew to encompass all dental materials and some equipment. His dedication to precision in all of his endeavors lead to Dr. Souder's being recognized as the 'Father of Dental Materials Research.' He became president of the International Association for Dental Research and an honorary member of the American College of Dentists and the American Dental Association. A short biography covers his early years and his education in physics at the University of Chicago. It also includes his many contributions to dental materials research and some of his many successes in criminology.

*601,335*
**PB86-209947** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Basic Alloys and Compositions.**
Final rept.,
J. A. Tesk. 1986, 13p
Pub. in Proceedings of International Workshop on Biocompatibility, Toxicity and Hypersensitivity to Alloys Systems Used in Dentistry, Ann Arbor, MI., June 23-25, 1985, p3-15 1986.

Keywords: *Dental alloys, Composition, Structure, Gold, Nickel, Cobalt, Chromium.

There are today a great number of dental alloys covering a wide range of compositions (Classification System for Cast Alloys, 1984; Tuccillo, 1977; and Dentists Desk Reference, 1983). Even with the exclusion of amalgams, the variety in composition and application is almost unlimited as indicated in Table 1.1 (Classification System for Cast Alloys, 1984; Jelenko Alloys, Composition Chart, 1984; Dentists Desk Reference, 1983; Tuccillo, 1977; Moffa, 1977; Hodges, 1977; Coleman, 1928; and Phillips, 1973).

*601,336*
**PB86-209970** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Adsorption of Benzoic Acid on Pure and Cupric Ion-Modified Hydroxyapatite: Implications for Design of a Coupling Agent to Dental Polymer Composites.**
Final rept.,
D. N. Misra. 1986, 6p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of Dental Research 65, n5 p706-711 May 86.

Keywords: *Adsorption, *Dental composites, Hydrogen bonding, Hydroxyapatite, Reprints, *Benzoic acid, Coupling agents.

The adsorption isotherms of benzoic acid on synthetic hydroxyapatite (containing about 1.5 monolayers of physisorbed water) were studied from ethanol, dimethylsulfoxide, p-dioxane, methylene chloride, and benzene to discern the role of solvent in the process. The adsorption is reversible from the first three solvents and follows the Langmuir plots. It is irreversible from the last two, and a constant amount of absorbent is removed from solutions above a certain concentration. The isotherms of potassium benzoate on the apatite from ethanol and dimethyl sulfoxide were reversible. The isotherms of the acid on cupric ion-modified apatite surfaces from ethanol and benzene were identical with those obtained on the pure hydroxyapatite. This may demonstrate that any 'surface chelation' with the cation may not be a significant factor for adsorption to occur.

*601,337*
**PB86-209988** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Recording Dilatometer for Measuring Polymerization Shrinkage.**
Final rept.,
R. W. Penn. 1986, 2p
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Dental Materials 2, p78-79 1986.

Keywords: *Dental composites, Dental cements, Reprints, *Dilatometer, *Polymerization shrinkage, Recording dilatometer.

The volumetric changes which occur during curing of dental resins and cements is considered important to

their clinical performance. To measure these changes a dilatometer device is required. A device is described in the literature (deGree and Davidson 1981) but its stability has been found to be worse (by a factor of ten) than conveniently acceptable. Using the same principles, a device with modified components and accessories and improved stability has been developed. It is constructed from the female part of a spherical glass joint which is ground flat and covered with a flat quartz plate. The stem of the joint is bent into a U-tube and filled with mercury. The height of the mercury in the U-tube is measured by a linear variable differential transformer which indicates volume changes in the sample which is placed in the joint on the bottom side of the quartz plate. The device is stable to 0.00001 cc over periods of several hours.

*601,338*
**PB86-231529** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Complexes of Iron Cations with N-Phenylglycinate or Oxalic Acid.**
Final rept.,
R. L. Bowen, and D. N. Misra. Mar 86, 5p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of Dental Research 65, n3 p412-416 Mar 86.

Keywords: *Oxalic acid, *Iron, Dentistry, Teeth, Dentin, Adhesion, Metal complexes, Reprints, *Glycine/N-phenyl, Tooth enamel.

N-phenylglycine plays a very important role in obtaining adhesion of restorative composites to dentin and enamel (Bowen et al., 1982a). In a systematic investigation, ferric or ferrous N-phenylglycinate complexes formed when aqueous ferric nitrate or ferrous chloride was combined with solutions of potassium N-phenylglycinate in stoichiometric proportions. The molal ratios of iron ion to N-phenylglycinate ion in each complex were confirmed by osmolality measurements with a freezing-point osmometer. The reaction of aqueous solutions of oxalic acid with ferric nitrate indicated formation of ferric oxalate complexes with a stoichiometry of Fe2(oxalate)3 in solution, using Job's method of continuous variations (1925;1928).

*601,339*
**PB87-122255** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Effects of Neutral Salts in a Bench-Scale Caries Model.**
Final rept.,
W. E. Brown, and L. C. Chow. 1986, 6p
Sponsored by American Dental Association Health Foundation, Chicago, IL., and Public Health Service, Rockville, MD.
Pub. in Jnl. of Dental Research 65, n9 p1115-1120 Sep 86.

Keywords: *Fluoride, Membranes, Sodium fluoride, Reprints, *Dental caries, Hydroxyapatite, Fluorapatite.

In an earlier paper on bench-scale simulation of the caries process, it was shown that the passage of ions through ion-permselective barriers could have profound effects on the composition of the solution within the 'lesion' at steady state. As indicated in earlier papers, these changes are produced by unequal rates of diffusion of Ca and PO4 ions prior to reaching steady state. Comparable effects are attributable to F ions when present. Here, the authors used the same two-compartment diffusion apparatus and membranes, as described in the earlier paper, to show that a neutral salt, such as NaCl, disproportionates under the influence of membrane potential. Thus, although the Na and Cl concentrations are nearly equal in the 'plaque-saliva' compartment, they become very different in the 'lesion' solution.

*601,340*
**PB87-122271** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Composite Resin Chemistry: The Effects of Solvents on Surface Hardness.**
Final rept.,
W. Wu, J. Pestaner, and R. L. Bowen. 1984, 14p
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Proceedings of the International Symposium on Posterior Composite Resins, Chapel Hill, NC., October 13-14, 1982, p7-20.

Keywords: *Sorption, *Dental materials, Surface properties, Solubility, Hardness, Softening, Swelling, Composite materials.

Nine liquid chemical compounds, with a solubility parameter range of 7.4 to 23.4 (Cal/cc)(sup 1/2), were used to study how sorption affects the properties of BIS-GMA co-polymers. One commercial dental restorative composite and one unfilled BIS-GMA resin were immersed in each of these chemicals. The changes in sample weight and surface hardness were monitored with time. No significant change in sample weight was observed over the test period of four weeks; however, a dramatic drop in hardness was found in both the composite and the unfilled resin after these materials were immersed in compounds with solubility parameters from 8.9 to 14.7 (Cal/cc)(sup 1/2).

## Pathology

*601,341*
**PB86-241734** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Accuracy of Particlpant Results Utilized as Target Values in the CAP Chemistry Survey Program.**
Final rept.,
A. E. Hartmann, H. K. Naito, R. W. Burnett, and M. J. Welch. Oct 85, 10p
Pub. in Archives of Pathology and Laboratory Medicine 109, p894-903 Oct 85.

Keywords: *Definitive methods, Surveys, Reprints, *Organic serum analytes.

Samples of lyophilized human serum were circulated to more than 7,000 participants in the College of American Pathologists chemistry survey program. The participants measured the concentrations of glucose, cholesterol, uric acid, and urea along with other constituents in the samples. Selected samples also were sent to the National Bureau of Standards (NBS) for analysis of these same analytes by definitive methods. Consensus mean values of participant results are used as target values.

*601,342*
**PB86-242179** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Journal of Research of the National Bureau of Standards, Volume 91, Number 2, March-April 1986.**
Apr 86, 74p
See also PB86-242187 through PB86-242245, and PB86-206364. Also available from Supt. of Docs as SN703-027-0009-1.

Keywords: *Tissues(Biology), *Sampling, Humans, *Biomedical sampling, Trace elements, Urinalysis, Neutron activation analysis.

Contents: Representative sampling of human tissue; Technical considerations for sampling and sample preparation of biomedical samples for trace element analysis; Environmental specimen banking; Presampling factors; The sampling and analysis of human livers; The collection and preparation of human blood plasma or serum for trace elements analysis; Storage and pre-neutron ativation analysis treatment for trace element analysis in urine.

*601,343*
**PB86-242187**
(Order as PB86-242179, PC **A04**/MF **A01**)
Medical Coll. of Ohio at Toledo.
**Representative Sampling of Human Tissue,**
H. C. Hopps. 24 Oct 85, 4p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p47-50 Mar-Apr 86.

Keywords: *Tissues(Biology), *Sampling, Qualtiy control, Analysis, *Biomedical sampling, Trace elements.

In the chemical analyses of tissues for trace elements, quality control of the tissue sample for its anatomic composition is a critically important step that is frequently overlooked. This is because the analyst often assumes a degree of homogeneity that does not exist. The means of attaining a representative sample vary greatly depending on the organ or tissue involved, and also on the level of resolution chosen, i.e., the size of the sample.

*601,344*
**PB86-242195**
(Order as PB86-242179, PC **A04**/MF **A01**)
International Atomic Energy Agency, Vienna (Austria).
**Technical Considerations for Sampling and Sample Preparation of Biomedical Samples for Trace Element Analysis,**
R. M. Parr. 24 Oct 85, 7p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p51-57 Mar-Apr 86.

Keywords: *Tissues(Biology), *Sampling, Analysis, Contamination, Quality assurance, Handling, *Biomedical sampling, *Trace elements.

Sampling and sample preparation procedures are to a large extent determined by the analytical method used since different methods vary in the amount of material required for analysis and in how this is pre-treated before being introdued into the measuring instrument. Judging from imtercomparison studies conducted by the International Atomic Energy Agency (IAEA), the most widely applicable methods now in use are Neutron Activation Analysis, Atomic Absorption Spectrometry, and Inductively Coupled Plasma Atomic Emission Spectrometry, though the latter still seems to have insufficient sensitivity for many trace elements of biomedical interest. Common to all thses methods is the problem of contaminating the sample before or during analysis. For many elements sufficient control over contamination can only be achieved by the use of special tools and reagents, and by working in a controlled (dust-free) environment. Several important elements are subject to losses on drying or ashing, but can be recovered reliably if wet-ashed in a closed container such as a PTFE 'bomb'. For representative sampling it is almost always necessary to start with several grams of material, and to homogenize this, if the effects of sample heterogeneity are to be reduced to an acceptable level. Quality assurance procedures covering all these aspects are difficult both to define and to apply. However, much can be learned from the statistical evaluation of results for duplicate samples, and from a determination of the limit of quantitation of the analytical procedure.

*601,345*
**PB86-242203**
(Order as PB86-242179, PC **A04**/MF **A01**)
Muenster Univ. (Germany, F.R.).
**Environmental Specimen Banking: The Selection, Collection, Transport, and Storage of Biomedical Samples,**
F. H. Kemper, and N. P. Luepke. 24 Oct 85, 7p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p59-65 Mar-Apr 86.

Keywords: Humans, Exposure, *Specimen banking, *Biomonitoring, *Biomedical sampling.

In order to adequately ensure the protection of human health and the environment from the thousands of presently suspected hazardous substances and the new compounds added to those by new industrial processes, sophisticated approaches to hazard assessment and monitoring are being established. Environmental specimen banking (ESB) is necessary, useful, and important for environmental monitoring currently, and in the future for monitoring the past. ESB has already proved a good tool for recording inorganic and/or organic pollution trends over the years. Moreover, ESB offers the possibilities and potentials for retrospective analysis of authentic samples from the past by improved futhure analytical procedures, including the detection of presently unnoticed environmental chemicals of biological interest. Among the specimens representing the environment, specimens of human origin play a key role. The selection criteria for human specimens include ethical and legal considerations together with the appropriate scientific approaches and epidemiological criteria. Technical considerations for sampling, preparation, transportation, and storage of the specimens include the selection and development of specific materials and implements, cold storage, and clean room technology in order not to compromise the original composition of the sample.

*601,346*
**PB86-242211**
(Order as PB86-242179, PC **A04**/MF **A01**)
Kernforschungsanlage Juelich G.m.b.H. (Germany, F.R.).
**Presampling Factors,**
G. V. Iyengar. 24 Oct 85, 8p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p67-74 Mar-Apr 86.

Keywords: *Tissues(Biology), *Sampling, Humans, *Biomedical sampling, *Trace elements.

Choosing the right kind of samples from human subjects for trace element studies poses many difficult problems. First of all, due to practical considerations, specimens with clinical relevance are restricted to a few such as whole blood, hair, nail, urine, and faeces. Although autopsies provide access to collect various organs, their usefulness is restricted to monitoring type of activities and not for clinical diagnosis. Besides these basic differences one is also confronted with procuring 'valid' samples for analysis. Validity refers to both analytical and biological aspects and the material collected should satisfy both the demands to make the specimen meaningful. In practice this is not a simple task because a number of presampling factors need to be taken into account. Significant situations among these are the biological variations, post mortem changes, intrinsic errors resulting from internal contaminations, etc. The impact of these factors alters the status of the sample and calls for adequate discription of the specimen. In the absence of a well defined sample protocol accurate characterization of the material will not be possible and renders the analytical effort worthless. Solutions to these problems should be sought at interdisciplinary level and effective team work is mandatory to make any meaningful progress in endeavors to answer public health questions.

*601,347*
**PB86-242229**
(Order as PB86-242179, PC **A04**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Sampling and Analysis of Human Livers,**
R. Zeisler. 9 Jan 86, 11p
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p75-85 Mar-Apr 86.

Keywords: *Liver, *Tissue preservation, *Sampling, Humans, Low temperatures, *Biomedical sampling, Trace elements, Neutron activation analysis.

A comprehensive approach to the analysis of human livers has been developed in a pilot program for a National Environmental Specimen Bank (NESB). Since 1980, the pilot NESB program has examined the collection, processing, storage and analysis of human livers. Sampling protocols, handling procedures and analytical methods have been developed and implemented considering the requirements for valid analytical results. Sampling and handling included the use of cleanroom technology, specific clean implements and packing materials made from titanium and Teflon and flash-freezing and preservation at liquid nitrogen scheme combined up to four analytical techniques to determine the distribution of 29 trace elements in 66 human livers.

*601,348*
**PB86-242237**
(Order as PB86-242179, PC **A04**/MF **A01**)
Ghent Rijksuniversiteit (Belgium).
**Collection and Preparation of Human Blood Plasma or Serum for Trace Element Analysis,**
J. Versieck. 24 Oct 85, 6p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n2 p87-92 Mar-Apr 86.

Keywords: *Blood collection, *Sampling, Reagents, Containers, Contaminiation, Humans, *Clean rooms.

Trace element concentrations in blood plasma or serum have been assayed by numerous investigators using a variety of analytial techniques. For serveral elements, figures obtained in different centers are widely disparate. Impressive evidence has accumulated that a great deal of the inconsistencies should be ascribed to unsuspected contamination of the samples with exogenous material during their collection and preparation. In the paper, a number of potential sources of extraneous additions are indicated. Methods for controlling contamination are also briefly discussed.

## Pharmacology & Pharmacological Chemistry

*601,349*
**PB87-128401** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Clinical Evaluation of a Hydroxyapatite Precipitate for the Treatment of Dentinal Hypersensitivity.**
Final rept.,
W. G. de Rijk, W. E. Brown, and L. C. Chow. 1986, 4p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Biomedical Engineering V Recent Developments, p336-339 1986.

Keywords: Hypersensitivity, Dicalcium phosphate dihydrate, Sensitivity, Reprints, *Dentin tubule, *Hydroxyapatite, Tetracalcium phosphate.

A newly developed paste that precipitates hydroxyapatite has been clinically evaluated for the treatment of dentinal hypersensitivity. Both the experimental paste and the placebo ($SnO_2$) produced a significant reduction in patient discomfort. Only a minor difference was observed in the paste over the placebo.

## Physiology

*601,350*
**PB87-113726** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
**Effects of Time-Varying Noise on Human Response: What Is Known and What Is Not.**
Final rept.,
S. L. Yaniv, and J. W. Bauer. 1980, 11p
Pub. in Proceedings of International Congress on Noise as a Public Health Problem, Freiberg (Germany, F.R.), September 25-29, 1980, p511-521.

Keywords: *Noise, *Responses, Humans, Time varying noise.

No abstract available.

## Public Health & Industrial Medicine

*601,351*
**NUREG/CR-3400** PC **A04**/MF **A01**
National Bureau of Standards (NML), Washington, DC. Center for Radiation Research.
**Analysis of Measurements with Personnel Dosimeters and Portable Instruments for Determining Neutron Dose Equivalent at Nuclear Power Plants.**
Final technical rept. Aug 81-Jun 83,
C. M. Eisenhauer, and R. B. Schwartz. Aug 83, 75p

Keywords: *Nuclear power plants, *Radiation dosage, *Dosimetry, Proportional counters, Gamma rays, Calibrating, Nuclear reactor containment, Portable equipment, *Neutron dosimetry, *Dose equivalents, Remmeters, Tissue-equivalent detectors.

Published data from measurements made by Pacific Northwest Laboratory (PNL) and those made jointly by the Environmental Measurements Laboratory (EML) and by Rensselaer Polytechnic Institute (RPI) inside containment at nuclear power plants were examined for the purpose of determining the best method for estimating the neutron dose equivalent received by workers. These data included measurements with TLD albedo dosimeters, 9-inch spherical remmeters, Andersson-Braun remmeters, multisphere sets, 'Cutie Pie' gamma survey meters, 3He spectrometers, and tissue equivalent proportional counters. Results are presented.

## Radiobiology

*601,352*
**PB86-193836** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Enhanced Sensitivity of Chemical Dosimeters Using Liquid-Core Optical Waveguides.**
Final rept.,
B. B. Radak, W. L. McLaughlin, and M. G. Simic. 1986, 6p
Pub. in Nuclear Instruments and Methods in Physics Research A243, p201-206 1986.

Keywords: *Chemical dosimeters, Fiber optics, Spectrophotometers, Absorption spectra, Reprints, Optical waveguides.

The spectrophotometric sensitivity of chromophoric chemical dosimeters can be enhanced by increasing the optical path length through the light absorbing medium. The approach is used with optical waveguide (OWG) dosimeters, consisting of liquid-phase light-propagating media filling the core of a long, thin flexible polymer tubing. The liquid phase consists of dimethyl sulfoxide, N, N,-dimet hylformamide, or triethyl phosphate solutions of hexa (hydroxyethyl) pararosaniline cyanide, a wellknown radiochromic dye precursor, which on irradiation converts from the leucoform into a brightly colored dye chromophore. The experimental design is described as well as the influences of some experimental parameters: length of the OWG, curvature of the waveguide loops, cross section of the liquid light-guiding core, the temperature and the solvent. It is suggested that such long OWG assemblies can be used for enhancing the response of chemical dosimeters for medical and radiation protection applications, as well as in analytical chemistry and for chemical kinetics studies.

*601,353*
**PB86-210085** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Use of Threshold Activation Detectors to Obtain Neutron Kerma for Biological Irradiations.**
Final rept.,
C. Eisenhauer, J. Grundl, C. Cassapakis, and V. Verbinski. 1985, 15p
Pub. in Reactor Dosimetry, p921-928 1985.

Keywords: *Neutron flux, Neutron spectra, Reprints, Benchmarks, Kerma, Activation detectors.

Fission and non-fission activation foils have been irradiated in experimental room at the Armed Forces Radiobiology Research Institute (AFRRI) in Bethesda, Maryland, in order to characterize the neutron field there. The field, which is generated by neutrons from a TRIGA MARK-F reactor adjacent to the room, is used for radiobiological experiments. Results from each of six activation detectors have been analyzed to estimate the absolute neutron kerma rate per unit power of the reactor. These kerma rates have been compared with those derived from tissue equivalent ionization chamber measurements, and with those calculated by the method of discrete ordinates. A few group neutron spectrum has been inferred from the activation measurements by means of a least-squares adjustment. An example is included of benchmark referencing to a fission neutron spectrum and consequent improvement in measurement confidence.

*601,354*
**PB86-230752** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Physics Div.
**Neutron Kerma Values.**
Final rept.,
R. S. Caswell, and J. J. Coyne. 1985, 3p
Pub. in Physics in Medicine and Biology Encyclopedia, p521-523 1985.

Keywords: Neutron irradiation, Reprints, *Kerma.

Kerma, K, is defined by the International Commission on Radiation Units and Measurements (ICRU) as the quotient of dE(tr) by dm, where dE(tr) is the sum of the initial kinetic energies of all the charged ionizing particles liberated by uncharged ionizing particles (such as neutrons) in a material of mass dm, that is $K = dE(tr)/dm$.

*601,355*
**PB86-242609** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Critical Evaluation of Neutron Kerma Factors Using Theoretical and Experimental Ionization Yield Spectra.**
Final rept.,
H. Schuhmacher, H. G. Menzel, and J. J. Coyne. 1984, 12p
Sponsored by Commission of the European Communities, Luxembourg, and Department of Energy, Washington, DC. Office of Health and Environmental Research.
Pub. in Symposium on Neutron Dosimetry (5th), Neuherberg, Germany, F.R., September 17-21, 1984, p213-224.

Keywords: Neutrons, Alpha particles, Proportional counters, *Neutron dosimetry, *Kerma, *Alpha dosimetry, Tissue-equivalent materials, MeV range 10-100, Carbon 12 target.

Ionization yield calculations were performed and compared to measurements for 13.9, 15.0, 17.0 and 19.0 MeV. The measured spectra were normalized to unit neutron fluence and the calculations take account of the neutron energy distributions at the detector positions. The computer code was tested by comparison with experimental data at 0.57, 2.07 and 5.25 MeV because physical data are well known at these energies. Total kerma for 19 MeV as well as kerma due to alpha-particles for 17.0 and 19.0 MeV are significantly lower for the measured data. There is clear evidence that the (12)C(n,n'3 alpha) cross section for 17 and 19 MeV used in the calculations and in kerma evaluations is too high.

*601,356*
**PB87-109872**
(Order as PB87-109864, PC **A05**/MF **A01**)
National Bureau of Standards, Gaithersburg, MD.
**Calibration of Beta-Particle Ophthalmic Applicators at the National Bureau of Standards,**
J. S. Pruitt. 27 Aug 86, 6p
Included in Jnl. of Research of the National Bureau of Standards, v91 n4 p165-170 Jul-Aug 86.

Keywords: *Opthalmology, *Calibrating, Strontium 90, Water, *Radiation doses, *Electron dosimetry, Yttrium 90.

The method used at the National Bureau of Standards for the calibration of strontium-90 + yttrium-90 beta-particle ophthalmic applicators in terms of absorbed dose to water, is described. The method involves measurement of ionization density at the applicator surface with an extrapolation chamber, correction for the difference in backscatter between the collection electrode and water, and application of the Bragg-Gray equation. The calibration obtained is an average over the active surface of the applicator. The overall uncertainty of the surface calibration is about + or - 15 percent.

*601,357*
**PB87-122552** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Future of A-150 TE Plastic.**
Final rept.,
L. J. Goodman. 1985, 16p
Pub. in Proceedings of Symposium on Neutron Dosimetry (5th), Munich, Neuherberg, Germany, September 17-21, 1984, v2 p687-694 1985.

Keywords: *Dosimetry, Plastics, Ionization chambers, *Tissue-equivalent materials, A 150 TE plastics, Neutron dosimetry.

The United States National Bureau of Standards is now considering the desirability of supplying A-150 plastic as a research material with at least the homogeneity certified. The authors are, however, faced with a dilemma since the nylon used in A-150 has been discontinued by the manufacturer and the current stock of A-150 has been estimated to be adequate to supply the demand for only the next 2 or 3 years. Thus, it will be necessary to reformulate the plastic mixture that will be used in the future. This may be a blessing in disguise because it offers the opportunity to change the composition of tissue-equivalent plastic to better conform to present-day requirements. To elucidate just what these requirements are, a postal survey of the opinions of neutron dosimetrists was conducted.

*601,358*
**PB87-130514** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**OH Radical-Induced Products of Tyrosine Peptides.**
Final rept.,
L. R. Karam, M. Dizdaroglu, and M. G. Simic. 1984, 10p
Pub. in International Jnl. of Radiation Biology 46, n6 p715-724 1984.

Keywords: *Tyrosine, *Peptides, Chemical reactions, Amino acids, Chemical radicals, Chromatographic analysis, Crosslinking, Chemical bonds, Reaction kinetics, Reprints, *Hydroxyl radicals, Phenoxy radicals.

Reactions of radiation-generated OH radicals with tyrosine and its homopeptides, i.e. L-Tyr-L-Tyr and L-Tyr-L-Tyr-L-Tyr, in N2O-saturated solutions were shown to give crosslinks between the peptide chains with high yields. High-performance liquid chromatography, capillary gas chromatography and mass spectrometry were used for isolation and identification of the monomeric and dimeric products. Evidence is presented for the crosslinking to occur through C - C and C - O - C bonds. Mechanisms of product formation are also discussed.

## Toxicology

*601,359*
**PB86-182284** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Polystyrenes: A Review of the Literature on the Products of Thermal Decomposition and Toxicity,**
J. L. Gurman, L. Baier, and B. C. Levin. Mar 86, 88p NBSIR-85/3277
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Polystyrene, *Decomposition, *Toxicology, Pyrolysis, Combustion products, Test methods, Fire safety, Literature surveys.

The current English literature through 1984 on the products of pyrolysis and combustion from polystyrenes and the toxicity of those products is reviewed. Among 57 compounds detected by chemical analyses of the thermal decomposition products produced under various atmospheric conditions (vacuum, inert, and oxidative), the main volatile component is the styrene monomer. Evidence is provided that the mass fraction of styrene increases with furnace temperatures at least through 500 C. At 800 C and above, the concentration of styrene decreases. In oxidative atmospheres, carbon monoxide (CO), carbon dioxide (CO2) and oxidative hydrocarbons are formed. The concentrations of CO and CO2 are a function of temperature and combustion conditions, i.e., greater amounts are produced in the flaming than in the nonflaming mode. Eleven different test procedures were used to evaluate the toxicity of the pyrolysis and combustion atmospheres of polystyrenes.

*601,360*
**PB86-193067** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Predicting Toxicity Using Computed Molecular Topologies: The Example of Triorganotin Compounds.**
Final rept.,
R. B. Laughlin, W. French, R. B. Johannesen, H. E. Guard, and F. E. Brinckman. 1984, 10p
Pub. in Chemosphere 13, n4 p575-584 1984.

Keywords: *Biocides, *Toxicology, Lethal dosage, Crabs, Organatins, Solubility, Molecular biology, Reprints, *Triorganotin, Computer applications, *Water pollution effects(Animals).

Thermodynamic properties of sparingly soluble organic molecules in water have been correlated with boiling points and toxicity, suggesting that appropriate physicochemical descriptions of molecular conformation or topology can provide similar predictors. The paper reports a novel alternative to previous applications of substituent structure-activity coefficients based on experimental kinetic or equilibrium data to predict solubility and toxicity. The authors have developed a combined computer program utilizing SAREA and PROPHET NET which, respectively, permit independent calculations of total available surface areas TSA of organometallic molecules based upon bond distances and angles, and expected conformations in aqueous media. Our first demonstration is applied to a comprehensive series of neurotoxic organotin compounds of commercial concern for which subacute LC50 toxicities toward crab larvae (Rhithropanopeus harrisii) in sea water were independently determined.

*601,361*
**PB86-201621** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Toxicity of the Pyrolysis and Combustion Products of Poly(vinyl chlorides): A Literature Assessment,**
C. Huggett, and B. C. Levin. Apr 86, 49p NBSIR-85/3286
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Polyvinyl chloride, *Combustion products, *Pyrolysis, *Toxicity, Plastics, Hazardous materials, Exposure, Lethal dosage, Air pollution, Hydrogen chloride, Carbon monoxide, Fire tests, Toxic substances, Inhalation, Indoor air pollution.

Poly(vinyl chlorides) (PVC) constitute a major class of synthetic plastics. Many surveys of the voluminous literature have been performed. The report reviews the literature published in English from 1969 through 1984 and endeavors to be more interpretive than comprehensive. PVC compounds, in general, are among the more fire resistant common organic polymers, natural or synthetic. The major products of thermal decomposition include hydrogen chloride, benzene and unsaturated hydrocarbons. In the presence of oxygen, carbon monoxide, carbon dioxide and water are included among the common combustion products. The main toxic products from PVC fires are hydrogen chloride (a sensory and pulmonary irritant) and carbon monoxide (an asphyxiant).

*601,362*
**PB86-210713** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Quantitative Determination of Smoke Toxicity Hazard - A Practical Approach for Current Use.**
Final rept.,
R. W. Bukowski. 1986, 12p
Pub. in Fire Safety Science--Proceedings of the First International Symposium, Gaithersburg, MD., pp. 1089-1100 (1986).

Keywords: *Toxicology, Hazardous materials, Validation, Statistical analysis, *Fire tests, *Smoke layers.

The concepts of fire hazard assessment are discussed. The development of these concepts into the framework for a hazard assessment model is described. This model, which is actually a group of interacting models, is presented in terms of the component functions and the interactions necessary to accomplish a hazard analysis. The most critical research issues which must be resolved in order to use this hazard analysis model for practical problems are identified. Preliminary results of experiments to assess the predictive accuracy of the multi-compartment transport model used within the hazard model are presented. A simple, engineering approach to toxicity evaluation included in the current model is also discussed.

*601,363*
**PB86-230679** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Summary of the NBS (National Bureau of Standards) Literature Reviews on the Chemical Nature and Toxicity of the Pyrolysis and Combustion Products from Seven Plastics: Acrylonitrile-Butadiene-Styrenes (ABS), Nylons, Polyesters, Polyethylenes, Polystyrenes, Poly(Vinyl Chlorides) and Rigid Polyurethane Foams,**
B. C. Levin. Jun 86, 37p NBSIR-85/3267
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Toxicology, *Pyrolysis, *Combustion products, *Plastics, Nylon, Polyesters, Polyethylenes, Polystyrenes, PVC, Polyurethane foams, Literature surveys, ABS.

A series of literature reviews was undertaken by the National Bureau of Standards to examine the toxicity and chemistry of the effluents produced when seven plastics were decomposed under various thermal and atmospheric conditions. These plastics are: acrylonitrile-butadiene-styrenes, nylons, polyesters, polyethylenes, polystyrenes, poly(vinyl chlorides), and rigid polyurethane foams. The English language literature on each of these was reviewed and published as a separate report of the National Bureau of Standards. Over 400 different thermal decomposition products, many common to more than one plastic, were identified. The toxicity of most of these individual products is unknown and an assessment of the toxicity of the multitude of possible combinations is not feasible at this time. Therefore, a variety of bioassay toxicity protocols have been used to assess the toxicity of the gaseous atmospheres generated by the thermal decomposition of these plastics. In general, these seven plastics did not produce unusually or extremely toxic pyrolysis or combustion products when compared to those of other synthetic or natural materials. In a few cases involving additives, toxic products of concern were produced.

*601,364*
**PB86-232303** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**Toxicity of the Combustion Products from a Flexible Polyurethane Foam and a Polyester Fabric Evaluated Separately and Together by the NBS (National Bureau of Standards) Toxicity Test Method.**
Final rept.,
B. C. Levin, M. Paabo, C. S. Bailey, and S. E. Harris. 1986, 12p
Sponsored by Consumer Product Safety Commission, Bethesda, MD.
Pub. in Proceedings of International Symposium on Fire Science Safety (1st), Gaithersburg, MD., October 7-11, 1985, p1111-1122 1986.

Keywords: *Toxicity, *Polyurethane resins, *Combustion products, Exposure, Fabrics, Rats, Ignition, Carbon monoxide, Hydrogen cyanide, *Toxic substances, *Polyester textiles, Inhalation, Lethal doses.

Representative specimens of two materials, a flexible polyurethane foam and a polyester, were thermally decomposed separately and together in order to compare the toxicological effects of the combustion products from the combined materials with those from the single homogeneous materials. Gas concentrations (CO, CO2, O2 and HCN), blood carboxyhemoglobin, and LC(50) values (the concentration of material necessary to kill 50% of the test animals (Fischer 344 male rats) during a 30 minute exposure and a 14 day post-exposure observation period) were determined for the separate and combined materials under both flaming and non-flaming conditions. The results of the combined experiments indicated that under non-flaming conditions, both materials contributed in an additive manner to the concentration of the combustion products. However, under flaming conditions, the generation of HCN and CO is greater than that predicted from the addition of the maximum amounts produced by the materials separately.

*601,365*
**PB87-140265** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Comparison of the Toxicity of the Combustion Products from a Flexible Polyurethane Foam and a Polyester Fabric Evaluated Separately and Together by the NBS (National Bureau of Standards) Toxicity Test Method and a Cone Radiant Heater Toxicity Test Apparatus,**
B. C. Levin, E. Braun, J. L. Gurman, and M. Paabo. Nov 86, 71p NBSIR-86/3457
Sponsored by Consumer Product Safety Commission, Washington, DC.

Keywords: *Toxicity, *Combustion products, *Foam, *Polyurethane resins, Concentration(Composition), Hydrogen cyanide, Rats, *Polyester fabrics, Toxicity test methods.

Representative specimens of flexible polyurethane foam and polyester fabric were thermally decomposed separately and together in order to compare the toxicity of the combustion products from the combined materials with those from the single homogeneous materials and to compare the toxicological results obtained with the NBS Toxicity Test Method with those using a cone radiant heater toxicity test apparatus. Gas concentrations (CO, CO2, O2 and HCN), blood carboxyhemoglobin, and LC(sub 50) values in Fischer 344 rats were determined for the materials under both flaming and non-flaming conditions. With the NBS Toxicity Test Method, the results of the non-flaming combined experiments indicated that both materials contributed in an additive manner to the concentration of the combustion products. However, under flaming conditions, the generation of HCN is greater than that predicted from the addition of the maximum amounts produced by the materials separately.

# MILITARY SCIENCES

## Logistics, Military Facilities, & Supplies

*601,366*
**PB87-118345** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
**Analytical Techniques for Military Construction Projects.**
Final rept.,
R. E. Chapman. 1984, 13p
Pub. in Proceedings of Symposium Operations Analysis in Cost Analysis, pII-122-II-134 1984.

Keywords: *Cost analysis, *Military facilities, Operation research, Construction cost.

The paper focuses on the theoretical and empirical considerations associated with the derivation, estimation and use of cost functions to control for variations in construction cost due to changing location and structure type. Regional factoring is used to develop a specific type of cost estimating relationship capable of estimating area cost factors for military construction projects. Accurate estimates of area cost factors are of crucial importance to the military since these factors are used as deflators to control for regional cost differentials among planned projects.

## Passive Defense Systems

*601,367*
**AD-P002 925/6** PC **A02**/MF **A01**
National Bureau of Standards (NEL), Washington, DC.
**Psychological Deterrents to Nuclear Theft,**
G. Lapinsky. 1 Jun 81, 5p
Pub. in Proceedings of the Symposium on the Role of Behavioral Science in Physical Security (5th Annual) Held at Gaithersburg, MD., June 11-12, 1980, AD-A138 882, p123-127.

Keywords: *Area security, *Deterrence, Management planning and control, Behavioral science, Social psychology, Threats, Crisis management, Component Reports, Physical security.

In 1975 the Defense Nuclear Agency (DNA) and the National Bureau of Standards jointly conceived the psychological deterrents project as an on-going review of the unclassified and the classified literature relating to psychological factors that may have impact on the design and development of DNA's Forced Entry Deterrent System (better known as FEDS). The classified and unclassified literature suggest that it may be possible to manipulate several human behavioral processes, but that there are few definitive data directly related to achieving deterrence by means of these psychological manipulations.

# NATURAL RESOURCES & EARTH SCIENCES

## Forestry

*601,368*
**PB86-234127** PC **A02**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
**Solid-State 13C NMR (Nuclear Magnetic Resonance) Determination of the Syringyl/Guaicyl Ratio in Hardwood,**
W. F. Manders. May 86, 23p NBSIR-86/3380

Keywords: *Lignin, *Hardwoods, *Softwoods, Nuclear magnetic resonance, Carbon isotopes, Decomposition, Oak trees, Spectrum analysis, Comparison, Nitrobenzenes, Oxidation reduction reactions, Syringylguaiacyl ratio.

The unprotonated aromatic regions of the solid-state 13C NMR spectra of several hardwoods and softwoods are examined. Spectra are acquired with cross polarization, magic-angle spinning, and delayed proton decoupling. The hardwood spectra are decomposed into syringyl and guaiacyl components with the aid of a softwood spectrum, which is assumed to be the same as the guaiacyl component of the hardwood spectrum. The molar ratio of syringylpropanoid units to guaiacylpropanoid units (S/G) in hardwood is determined from the intensities of their respective component spectra. These results were comparable to literature values that were obtained by a combination of methoxyl and elemental analyses.

## Geology & Geophysics

*601,369*
**PB86-160991** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Sawtooth Segmentation and Deformation Processes on the Southern San Andreas Fault, California.**
Final rept.,
R. Bilham, and P. Williams. 1985, 4p
Sponsored by Geological Survey, Reston, VA., National Aeronautics and Space Administration, Washington, DC., and National Geophysical Data Center, Boulder, CO.
Pub. in Geophysical Research Letters 12, n9 p557-560 Sep 85.

Keywords: *San Andreas Fault, *Geological faults, Earthquakes, California, Reprints.

Five continuous 12-13 km fault segments form a sawtooth geometry on the southernmost San Andreas fault. The kinematic and morphologic properties of each segment depend on fault strike, despite differences of strike between segments of as little as 3 degrees. Oblique slip (transpression) of fault segments within the Indio Hills, Mecca Hills, and Durmid Hill results from an inferred 8:1 ratio of dextral slip to convergence across the fault zone. Triggered slip and creep are confined almost entirely to transpressive segments of the fault. Durmid Hill has been formed in the last 28 + or - 6 ka by uplift at an average rate of 3 + or - 1 mm/a.

*601,370*
**PB86-193182** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**g -- The Acceleration of Gravity: Its Measurement and Its Importance.**
Final rept.,
I. Marson, and J. E. Faller. 1986, 11p
Pub. in Jnl. of Physics E: Scientific Instruments 19, p22-32 1986.

Keywords: *Gravitation, *Gravity, Measurement, Reprints.

The measurement of the acceleration of gravity (g) has long been a matter of scientific interest. Its value is of interest in a broad area of physical sciences, namely metrology, geophysics and geodesy. In the paper the authors discuss the various types of instrument, the methods of measurement, and the applications of g.

*601,371*
**PB86-200458** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
**Characterization of Polycyclic Aromatic Hydrocarbon Minerals Curtislte, Idrialite and Pendletonite Using High-Performance Liquid Chromatography, Gas Chromatography, Mass Spectrometry and Nuclear Magnetic Resonance Spectroscopy.**
Final rept.,
S. A. Wise, R. M. Campbell, W. R. West, M. L. Lee, and K. D. Bartle. 1986, 19p
Pub. in Chemical Geology 54, p339-357 1986.

Keywords: *Aromatic polycyclic hydrocarbons, Chemical analysis, Minerals, Gas chromatography, Mass spectroscopy, Nuclear magnetic resonance, Reprints, *Curtisite, *Idrialite, Liquid column chromatography.

Two polycyclic aromatic hydrocarbon (PAH) minerals-curtisite and idrialite-have been characterized using high-resolution gas chromatography-mass spectrometry (GC-MS) and high-performance liquid chromatography (HPLC) with fluorescence detection. Using analytical techniques, the curtisite and idrialite were found to be unique complex PAH mixtures consisting of six specific PAH structural series with each member of a series differing from the previous member by addition of another aromatic ring. The curtisite and idrialite samples contained many of the same components but in considerably different relative amounts. The identification of these compounds supports the conclusions of M. Blumer that these minerals were formed by medium-temperature pyrolysis of organic compounds, followed by extended equilibration at elevated temperatures in the subsurface.

*601,372*
**PB86-212842** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**GPS (Global Positioning System) Carrier Phase Ambiguity Resolution Over Long Baselines.**
Final rept.,
P. L. Bender, and D. R. Larden. May 85, 5p
Pub. in Proc. Int. Symp. on Precise Positioning with the Global Positioning System (1st), Rockville, MD., April 15-19, 1985, p357-361.

Keywords: *Geodesy, Navigation satellites, Carriers, Phase measurement, Resolution, Satellite orbits, *Global positioning systems.

As GPS satellite orbit determination accuracy improves, carrier phase ambiguity resolution over baselines 100 km to 1000 km or more in length will be desirable. With phase delay single differences for both the L1 and L2 frequencies from the j-th satellite, two particularly useful linear combinations can be formed. One is dj, a measure of the difference in geometric distance to the ground stations plus the clock correction. The other is gj, a measure of the difference in integrated electron content along the two paths. The information should make possible ambiguity resolution over long baselines if the orbits, phase measurements, and tropospheric corrections are sufficiently accurate.

*601,373*
**PB86-228657** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Geophysical Reasons for Monitoring Contemporary Plate Motions and the Earth's Rotation.**
Final rept.,
P. L. Bender. 1983, 5p
Pub. in Proceedings of Workshop on Multiple Uses of the Very Long Baseline Array, Washington, DC., April 8-9, 1983, p39-43.

Keywords: Polar wandering, Earthquakes, *Plate tectonics, Earth rotation, Plates (Tectonics), Very long base interferometry.

A number of types of scientific information which can be expected from studies of present tectonic plate motions, distortions in seismic zones, polar motion, and changes in the Earth's rotation rate are described. Contributions which could be made by the Very Long Baseline Array through intensive observations after large earthquakes, and through regular monitoring during calibration periods, are emphasized.

*601,374*
**PB87-106076** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Effect of Fluorine on Viscosities in the System Na2O-Al2O3-SiO2.**
Final rept.,
D. B. Dingwell, C. M. Scarfe, and D. J. Cronin. 1985, 8p
Sponsored by Alberta Univ., Edmonton. Dept. of Geology.
Pub. in American Mineralogist 70, n1-2 p80-87 1985.

Keywords: *Fluorine, *Viscosity, *Slags, Silicate minerals, Albite, Reprints, *Silicates, Jadeite, Nepheline.

The effect of fluorine on melt viscosities of five compositions in the system Na2O-Al2O3-SiO2 has been investigated at one atmosphere and 1000-1600 deg C by concentric-cylinder viscometry. The compositions chosen were albite, jadite and nepheline on the join NaAlO2-SiO2 and two others off the join at 75 mole percent SiO2, one peralkaline and one peraluminous. All melt viscosities were independent of shear rate over two orders of magnitude, indicating Newtonian behavior. All viscosity-temperature relationships were Arrhenian within error. Fluorine reduces the viscosities and activation energies of all melts investigated.

*601,375*
**PB87-107116** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Theoretical Analysis of Chemical and Magnetic Ordering in the System Hematite-Ilmenite (Fe203-FeTi03).**
Final rept.,
B. P. Burton. 1985, 9p
Pub. in American Mineralogist 70, n9-10 p1027-1035 1985.

Keywords: *Order disorder transformations, Phase diagrams, Phase transformations, Thermodynamic properties, Metaliferous minerals, Entropy, Enthalpy, Reprints, *Hematite, *Ilmenite, Magnetic ordering.

A theoretical model of equilibrium phase relations in the system Fe2O3 FeTiO3 is presented. This model is based on the single prism approximation in the cluster variation method and includes both chemical and magnetic contributions to the free energy of mixing. The inclusion of a magnetic degree of freedom, and magnetic interaction parameters, leads to a more realistic treatment of the configurational entropy of mixing, and therefore, to improved estimates of the oxidation-reduction and cation-ordering contributions to the enthalpy of stabilization of FeTiO3 (relative to mechanical mixing of Fe2O3 and Ti2O3). Two tricritical points are predicted to occur in the Fe2O3 - FeTiO3 phase diagram: one at which an Fe-Ti order-disorder transition pierces the peak of a two-phase field; and a second at which the two phase field is intersected by an essentially antiferromagnetic transition. Below this latter point, the two-phase field is predicted to bulge out (towards Fe2O3) and it is argued that this feature should be useful in geothermometry.

*601,376*
**PB87-118584** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Absolute Gravity: A Reconnaissance Tool for Studying Vertical Crustal Motions.**
Final rept.,
T. M. Niebauer, J. K. Hoskins, and J. E. Faller. 1986, 5p
Sponsored by Air Force Geophysics Lab., Hanscom AFB, MA., and Defense Mapping Agency, Washington, DC.
Pub. in Jnl. of Geophysical Research 91, nB9 p9145-9149, 10 Aug 86.

Keywords: *Gravimeters, *Tectonics, Portable equipment, Gravity, Reprints.

A major effort is under way to develop highly portable absolute gravimeters having an ultimate accuracy of 3-5 microGal, an accuracy which translates into a height sensitivity of several centimeters. The authors are just finishing the construction of six such units. Measurements at the Joint Institute for Laboratory Astrophysics with one of these new instruments agree well with the earlier measurements made in 1981 and 1982 with a previous generation instrument. Recent measurements at the International Bureau of Weights and Measures in Sevres, France, as a part of an international intercomparison of absolute gravimeters, also show good agreement with the other instruments.

*601,377*
**PB87-134219** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Densely Spaced Array of Sea Level Monitors for the Detection of Vertical Crustal Deformation In the Shumagin Seismic Gap, Alaska.**
Final rept.,
J. Beavan, K. Hurst, R. Bilham, and L. Shengold. 1986, 14p
Pub. in Jnl. of Geophysical Research 91, nB9 p9067-9080, 10 Aug 86.

Keywords: *Earthquakes, *Shumagin Island, Monitoring, Earth crust, Motion, Sea level, Pressure gages, Deformation, Alaska, Reprints, Tiltmeters.

The authors have installed a network of sea level gauges with approximately 40 km spacing in the Shumagin Islands in order to detect relative vertical motion, in particular, possible crustal motion precursory to an expected major earthquake. This required the development and deployment of a pressure sensor sea level gauge suitable for installation on remote and harsh coastlines. Data are collected in near-real-time via satellite, both in order to exploit fully any precursors that may be observed and to provide continuous information on the status of the instruments. Using Wiener filtering techniques, the authors have determined conservatively that no relative vertical crustal motion greater than 0.1 m between stations has occurred during 1981-1985. A short-baseline tiltmeter operating in a tunnel has demonstrated that suitably designed and located land-based tiltmeters have a lower noise level, and hence better precursor detection characteristics than the sea level gauges, at monthly and shorter periods.

*601,378*
**PB87-135018** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Hydrostatic Levels in Precision Geodesy and Crustal Deformation Measurement.**
Final rept.,
K. Hurst, and R. Bilham. 1986, 15p
Grant NSF-EAR81-16369
Sponsored by National Science Foundation, Washington, DC., and National Geodetic Survey, Rockville, MD.
Pub. in Jnl. of Geophysical Research 91, nB9 p9202-9216, 10 Aug 86.

Keywords: *Geodesy, Precision, Reprints, *Hydrostatic leveling.

Previous attempts to apply the principles of hydrostatic leveling to precision geodesy have been limited by the uniformity of the fluid density attainable in field environments. This is largely due to the effects of temperature variations in the fluid tube. The authors have overcome this difficulty by using water maintained near its maximum density at 3.98 C inside a counterflow heat exchanger to limit the variations in density to less than 1 ppm. They have demonstrated the feasibility of this method with a 14-m prototype level and have used a computer model of the system to demonstrate the theoretical performance of instruments up to 1 km long. It appears possible, for example, to construct a fluid tube 200 m long, 12.5 cm in diameter, and weighing 3.8 kg/m that would provide uniform density to $< 1$ ppm in field environments between -40 and 50 C. In their attempt to use the 14-m prototype pressure-transfer level they were unable to exploit the density stability that they had achieved due to inadequacies in available pressure gauges.

## Mineral Industries

*601,379*
**PATENT-4 618 410** Not available NTIS

Department of Commerce, Washington, DC.
**Shale Oil Dearsenation Process.**
Patent,
F. E. Brinckman, T. F. Degnan, and C. S. Weiss.
Filed 4 Nov 85, patented 21 Oct 86, 5p PB87-113676, PAT-APPL-6-794 590
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Patents, *Shale oils, Coking, *Dearsenation process, PAT-CL-208-97.

An improved process for shale oil dearsenation comprises coking a retorted shale oil stream following by contacting the liquid coker product with water. Water washing is preferably carried out under ambient conditions to achieve a reduction to less than 3 ppm w soluble arsenic.

*601,380*
**PB87-103271** PC **A07/MF A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Development of a Fire Evaluation System for Underground Coal Mines,**
J. A. Shibe. Aug 86, 146p NBSIR-86/3425
Sponsored by Bureau of Mines, Pittsburgh, PA.

Keywords: *Coal mines, *Fire safety, Fire hazards, Fire protection, Underground mining, Evaluation.

A prototype Fire Safety Evaluation System has been developed and is ready to be evaluated by a Peer Consulting Panel and for performing field tests. The system can be used to determine combinations widely accepted fire safety equipment and underground coal mines features that provide a level of safety equivalent to those required by the Code of Federal Regulations-Title 30 for underground coal mines. In this evaluation, equivalent safety performance is gauged in terms of overall level of safety provided rather than by a component by component comparison.

*601,381*
**PB87-117941** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Water Sprays Suppress Gas-Well Blowout Fires.**
Final rept.,
D. Evans, and D. Pfenning. 1985, 7p
Pub. in Oil and Gas Jnl. 83, n17 p80-86 1985.

Keywords: *Blowouts, *Fire fighting, *Gas wells, Spraying, Oil wells, Fire extinguishing agents, Fires, Reprints, *Water sprays.

No abstract available.

*601,382*
**PB87-127981** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Crystal Structures of Boblerrite and Synthetic Mg3(PO4)2 . 8H2O.**
Final rept.,
S. Takagi, M. Mathew, and W. E. Brown. 1986, 5p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in American Mineralogist 71, p1229-1233 1986.

Keywords: *Crystal structure, Hydrates, Minerals, Reprints, *Bobierrite, *Vivanite, *Magnesium phosphate octahydrate.

The crystal structures of two forms of Mg3(PO4)2.8H2O, bobierrite (I) and the synthetic polymorph (II), have been determined by single-crystal X-ray diffraction. Crystal data for polymorph I are space group C2/c, a=4.667(1), b=27.926(8), c=10.067(3) A, beta=105.01(2), Z=4, R=0.041 for 963 reflections. Crystal data for polymorph II are space group C2/m, a=10.034(1), b=13.407(2), c=4.657(1) A, beta=105.09(1), Z=2, R=0.025 for 510 reflections. The structure of polymorph I is closely related to that of the vivianite group, whereas polymorph II is isostructural with vivianite. Both structures consist of octahedral edge-sharing dimers Mg2O6(H2O)4 and independent MgO2(H2O)4 octahedra linked together by PO4 tetrahedra to form complex sheets parallel to (010). The arrangement of these sheets along b is different in the two structures.

*601,383*
**PB87-134318** PC **A04/MF A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Momentum Diffusion Flame Characteristics and the Effects of Water Spray,**
B. J. McCaffrey. Nov 86, 72p NBSIR-86/3442
Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Fire safety, *Blowouts, Diffusion flames, Extinguishing, Model tests, Spraying, Water, *Natural gas wells, Blow off.

For water spray suppression of gas well blowout fire applications, reasonably large scale (1-10 MW) methane diffusion flames have been investigated near the high Froude number limit. Flame blow-off has been observed with pipe sizes to 30 mm diameter. Flame and lift-off heights, centerline temperatures and incident radiative flux to nearby targets have been measured with and without water spray suppressant. Using the Dayan-Tien formulation for a cylindrical flame model an effective gray absorption coefficient approaching 0.2/m was determined at the blow-off limit. The derived shape of the functional dependence of decreasing radiative fraction with jet Froude number in the limit is consistent with small scale experiments. The effect of spraying water internal to the flame envelope at the base is to shift or raise the flame above its normal position and to lower peak flame temperature and radiation levels despite increased absorptivity due to the radiatively active steam. Extinguishment near blowoff is thought due to the former effect. Calculations of flame entrainment based on increased water vapor emission are consistent with literature estimates of entrainment when account of the effects of buoyancy due to the liquid spray is provided.

# NAVIGATION, GUIDANCE, & CONTROL

## Navigation & Guidance System Components

*601,384*
**PB87-106779** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
**Naval Observatory Time Dissemination before the Wireless.**
Final rept.,
I. R. Bartky. 1983, 28p
Pub. in Proceedings of the Sesquicentennial Symposia of the U.S. Naval Observatory 'Sky with Ocean Joined', Washington, DC., December 5-8, 1980, p1-28 1983.

Keywords: *Time standards, Chronometers.

An historical outline of USNO time dissemination services prior to radio is presented. The various needs for accurate, such as for longitude determinations, for the general public, and for sea navigation are mentioned. The talk emphasizes the development and deployment of visual time signals, or time balls, for rating ship chronometers.

## Navigation Systems

*601,385*
**PB87-111654** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Weighting and Smoothing of Data in GPS Common View Time Transfer.**
Final rept.,
M. A. Weiss. 1986, 16p
Pub. in Proceedings of Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (17th), Washington, DC., December 3-5, 1985, p261-276 1986.

Keywords: Data smoothing, *Global positioning systems, *Time transfer.

It is now possible to compare a clock with UTC(NBS) anywhere in common view of a GPS satellite with Boulder, Colorado at the full level of accuracy and stability of the NBS atomic time scale for integration times of about four days and longer via the NBS Global Time Service. The availability includes Japan, Europe, and the entire United States. The service includes a dial-up service for current estimates of the user's clock performance, and a monthly report with improved estimates after the fact. The authors discuss here the exact method by which the common view time transfer values in the monthly reports are computed.

# NUCLEAR SCIENCE & TECHNOLOGY

## Fusion Devices

*601,386*
**PB86-231099** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Development of Radiation-Resistant Organic Insulators for Magnetic Fusion Energy Applications.**
Final rept.,
M. B. Kasen. 1985, 4p
Sponsored by Department of Energy, Washington, DC. Div. of Magnetic Fusion Energy.
Pub. in Proceedings of International Conference on Nuclear Power Plant Aging, Availability Factor and Reliability Analysis, San Diego, CA., July 8-12, 1985, p265-268.

Keywords: *Electrical insulation, Superconducting magnets, Neutron irradiation, Cryogenics, *Physical radiation effects, Gamma radiation, Fusion reactors.

Current knowledge of cryogenic irradiation effects on organic-matrix electrical insulators required for the superconducting magnets in magnetically-confined, fusion energy systems is reviewed. It is concluded that the performance of presently available materials is marginal for such applications. Since the cost of substituting inorganic materials as insulators appears to be inordinately expensive, a program to develop organic insulators having improved performance is under way. The program will make use of the National Low Temperature Neutron Irradiation Facility currently being constructed at ORNL. The main features of the program are described.

*601,387*
**PB86-243375** PC **A15/MF A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Materials Studies for Magnetic Fusion Energy Applications at Low Temperatures - 9.**
Technical rept.,
R. P. Reed. May 86, 333p NBSIR-86/3050
See also PB85-236362. Sponsored by Department of Energy, Washington, DC. Office of Fossil Energy.

Keywords: *Superconducting magnets, *Stainless steels, Cryogenics, Copper, Aluminum, Weldments, Mechanical properties, Toughness, Fusion reactors, Steel 316, Steel 304, Steel 308, Fiber reinforced composites, Physical radiation effects.

The report contains results of a research program to produce material property data that will facilitate design and development of cryogenic structures for the superconducting magnets of magnetic fusion energy power plants and prototypes. Research results for 1985 are summarized in an initial 'Highlights of Results' section and reported in detail in the technical papers that form the main body of the report. The technical papers are presented under four headings reflecting the main program areas: Welding, Nonmetallics, Structural Alloys, and Technology Transfer. Objectives, approaches, and achievements are summarized in an introduction to each program area.

## Fusion Devices

*601,388*
**PB87-128971** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Strategy for the Data Base Construction on Radiation-Resistant Cryogenic Composite Insulators for Magnetic Fusion Energy Applications.**
Final rept.,
M. B. Kasen. 1986, 7p
Sponsored by Department of Energy, Washington, DC. Div. of Magnetic Fusion Energy.
Pub. in Proceedings of International Symposium on Fundamental Research Strategy in the Development of New Materials for Efficient Energy Conversion, Osaka (Japan), August 25-27, 1986, p112-118.

Keywords: *Superconducting magnets, *Electrical insulation, Fiber composites, Cryogenics, Fracture strength, Neutron irradiation, Fusion reactors, Data bases, Physical radiation effects, International cooperation.

A strategy is suggested for the development of fiber-reinforced, organic insulators to be used in superconducting magnets for magnetic fusion energy power systems. Two data bases are required. The first is a component data base providing information for basic materials selection. The second is an engineering data base generated on insulators fabricated from the selected components. Successful completion of these tasks requires multidisciplinary expertise. Cooperative research is presently under way among laboratories in the United States, Japan, and England.

## Isotopes

*601,389*
**PB87-105821** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Radiocarbon Dating of Microgram Samples: Accelerator Mass Spectrometry and Electromagnetic Isotope Separation.**
Final rept.,
L. A. Currie, G. A. Klouda, D. Elmore, and H. E. Gove. 1985, 6p
Pub. in Nuclear Instruments and Methods in Physics Research B12, n3 p396-401 1985.

Keywords: *Radiocarbon dating, Mass spectroscopy, Carbon 14, Electromagnetic isotope separation, Reprints, *Isotope dating, Standard reference materials.

An exploratory experiment was performed to investigate methods for extending the direct atom counting technique to natural radiocarbon samples containing only micrograms of carbon. A threefold approach was adopted for the study: direct measurement of a microgram-size sample, in the form of elemental carbon; dilution of a few micrograms of an environmental (atmospheric particulate) reference sample with inert ('dead') carbon; and implantation of carbon ions (as CO(1+)) into copper foil prior to placement in the tandem accelerator ion source. The last experiment, which linked work with the NBS variable-geometry electromagnetic isotope separator and the NSRL tandem Van de Graaff, automatically led to isotopic enrichment during the implantation step. All three phases of the experiment were unique (not previously attempted) and gave consistent results, indicating great promise for the future application of direct atom counting to individual trace chemical species of environmental or archaeological importance.

*601,390*
**PB87-108544** PC **A06**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
**Uranium-235 Isotope Abundance Standard Reference Materials for Gamma Spectrometry Measurements.**
Final rept.,
B. S. Carpenter, J. W. Gramlich, R. R. Greenberg, L. A. Machlan, and P. DeBievre. Sep 86, 101p NBS/SP-260/96
Also available from Supt. of Docs as SN003-003-02763-4. Library of Congress catalog card no. 86-600585. Prepared in cooperation with Commission of the European Communities, Geel (Belgium). Central Bureau for Nuclear Measurements, and Department of Energy, Argonne, IL. New Brunswick Lab.

Keywords: *Uranium 235, *Gamma ray spectroscopy, *Standards, Isotope availability, *Standard reference materials, Uranium oxides U308.

The accurate determination of isotope abundances by any method requires that the measuring systems be calibrated using well characterized isotope reference materials. The National Bureau of Standards (NBS) and the Central Bureau for Nuclear Measurements (CBNM) have jointly produced and certified U3O8 nondestructive assay (NDA) reference samples to be used for calibrating gamma measurements. Five different uranium abundances have been certified (0.31, 0.71, 1.95, 2.95, and 4.46 nominal mass percent, (235)U/U). In the 260 series publication, the material fabrication and certification are described and a discussion of the measurement results affecting the accuracy of gamma spectrometry is given. These certified standards represent the first example of an international effort that establishes traceability to NBS, CBNM, and the basic SI units.

## Nuclear Instrumentation

*601,391*
**DE85014352** PC **A02**/MF **A01**
British Columbia Univ., Vancouver. TRIUMF Facility.
**FASTBUS for the Particle Accelerator Laboratories.**
W. K. Dawson, L. Costrell, H. Ikeda, P. J. Ponting, and H. V. Walz. May 85, 3p SLAC-PUB-3697, CONF-850504-189
Contract AC03-76SF00515
Particle accelerator conference, Vancouver, Canada, 13 May 1985.
Also Pub. in IEEE Transactions on Nuclear Science NS-32, n5 p2089-2091 October 1985.

Keywords: *Accelerator Facilities, *Fastbus System, Data Acquisition Systems, Reviews, Specifications, ERDA/440104.

The FASTBUS modular high speed data acquisition and control system for high energy physics and other applications was described by Costrell and Dawson at the 1983 Particle Accelerator Conference. Both the specification and the implementation of this interlaboratory development have progressed considerably since that time. Because of its many attractive features, FASTBUS is currently in use in several major nuclear and high energy physics laboratories and is also finding application in other areas. 10 refs. (ERA citation 10:037526)

*601,392*
**NUREG/CR-4266** PC **A05**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Standard Beta-Particle and Monoenergetic Electron Sources for the Calibration of Beta-Radiation Protection Instrumentation.**
Technical rept. (Final) Sep 82-May 85,
M. Ehrlich, J. S. Pruitt, C. G. Soares, C. E. Dick, and H. T. Heaton. Aug 85, 85p NBSIR-85-3169
Sponsored by Nuclear Regulatory Commission, Washington, DC. Office of Nuclear Regulatory Research.

Keywords: *Standards, *Calibrating, Radiation protection, Ionization chambers, Dose rate, *Beta sources, *Beta dosimetry, Electron sources, Beta detection, KeV range 100-1000, MeV range 01-10, Calibration standards.

In a project funded jointly by the National Bureau of Standards (NBS) and the Nuclear Regulatory Commission (NRC), NBS has developed a calibration facility for beta-particle instruments and sources used in radiation-protection dosimetry. The facility consists of beta-particle and nearly monoenergetic electron beams characterized in terms of absorbed-dose rates to plastic and in terms of beta-particle spectra. A second phase of the project was concerned with establishing secondary calibration laboratories for radiation-protection instruments. The final report includes a detailed discussion of (1) the determination of absorbed-dose rates to plastic for each beta-particle and nearly monoenergetic electron beam, dose-rate dependence on altitude above sea level, and an estimate of the overall uncertainties in dose-rate measurements; (2) beta-particle and nearly monoenergetic electron spectra and their dependence on source configuration; and (3) degree of achievable uniformity of beam cross sections. Included also is a review of the results of a first attempt to predict instrument response to realistic beta-particle environments from their response to monoenergetic electrons and knowledge of the approximate beta-particle spectra. Attached to the report are proposed guidelines for establishing secondary calibration laboratories for radiation-protection instruments.

*601,393*
**PB86-200748** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.
**New Two-Dimensional Position Sensitive Proportional Counter.**
Final rept.,
P. L. Cowan. 1986, 3p
Pub. in Nuclear Instruments and Methods in Physics Research A242, p484-486 1986.

Keywords: *Proportional counters, Photodiodes, Reprints, Microchannel electron multipliers, X-ray detection, Two dimensional, Position sensitive detectors.

A new scheme for two-dimensional position encoding has been devised for position sensitive proportional counters (PSPC). The method involves charge division at the cathode of the detector, similar to the 'wedge and strip' approach. The intrinsic spacial resolution of the encoding scheme suggests the possibility of applying the scheme to other two-dimensional detectors, such as micro-channel plates or photodiodes.

*601,394*
**PB86-210044** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Two-Dimensional PSD (Position Sensitive Detection) at the National Bureau of Standards' Small-Angle Neutron Scattering Facility.**
Final rept.,
C. J. Glinka, and N. F. Berk. 1983, 8p
Pub. in Proceedings of the Workshop on Position Sensitive Detection of Thermal Neutrons, Grenoble (France), October 11-12, 1982, p141-148 1983.

Keywords: Neutron scattering, Data acquisition, *Position sensitive detectors, *Neutron detectors, Two dimensional, Small angle scattering.

A new facility for small-angle neutron scattering (SANS) has been in operation at the NBS research reactor for about one year. The neutron detector at the NBS facility is the first commercial version of the Borkowski-Kopp type, 65 x 65 sq cm, PSD which was developed for use at the SANS facility at ORNL. The counter is based on RC-encoding and time-difference decoding of the positions of individual neutrons captured in the detector. In this article, measurements of the operating characteristics of the PSD, including linearity, spatial and energy resolution, uniformity, count rate capability, gamma ray sensitivity, and long-term stability, are presented. In addition, the position decoding electronics, which minimize the use of analog signal processing circuitry, are described.

*601,395*
**PB86-229697** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Physics Div.
**Measurement of the NBS (National Bureau of Standards) Black Neutron Detector Efficiency at 2.3 MeV.**
Final rept.,
K. C. Duvall, A. D. Carlson, and O. A. Wasson. 1985, 6p
Pub. in International Atomic Energy Agency (IAEA) Advisory Group Meeting on Nuclear Standard Reference Data, Geel, Belgium, November 12-16, 1984, p332-337 1985.

Keywords: Neutron flux, Efficiency, *Neutron detectors, MeV range 01-10.

The absolute efficiency of the National Bureau of Standards (NBS) Black Neutron Detector at 2.3 MeV has been measured using the time-correlated associated particle method. The measurement extends the usefulness of the Black Neutron Detector as an absolute neutron flux monitor to the higher energy region.

*601,396*
**PB86-232725** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

**Measurements of Inelastic Neutron Scattering in the eV Range.**
Final rept.,
C. D. Bowman, and R. G. Johnson. 1983, 7p
See also PB83-143818.
Pub. in Proceedings of Workshop on Thermal Reactor Benchmark Calculations, Techniques, Results, Applications, Upton, NY., May 17-18, 1982, p7-1 - 7-7 1983.

Keywords: *Neutron scattering, Inelastic scattering, Molecular vibrations, Excitation, eV range, Time-of-flight method.

The increasing availability of pulsed spallation neutron sources such as WNR at Los Alamos National Laboratory and IPNS at Argonne National Laboratory, has spurred interest in studies using epithermal neutrons. Among these are measurements of inelastic neutron scattering in the eV energy range. Such research offers the possibility of studying high-lying molecular rotational-vibrational states, atomic and molecular electronic excitations, and measurements of scattering laws at higher energies. In this paper the emphasis will be primarily on the methods used in measuring inelastic neutron scattering (in the eV region), where at NBS the first measurements of this kind have recently been performed. Emphasis will also be placed on interpretation of these inelastic scattering spectra and the implications to the problems of neutron moderation.

*601,397*
**PB86-239415** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**New Two Dimensional Position Sensitive Proportional Detectors Using Charge Division.**
Final rept.,
G. G. Luther, P. L. Cowan, A. Henins, and S. Brennan. 1986, 4p
Pub. in Nuclear Instruments and Methods in Physics Research A246, p537-540 1986.

Keywords: *Proportional counters, Reprints, *Position sensitive detectors, Two dimensional.

Several two dimensional position sensitive proportional counters have been built. The cathodes can encode the position of the event in one or two dimensions using capacitative charge division techniques; a backgammon configuration encodes in one dimension with anode encoding of the second dimension or a new cathode pattern can be used to encode in two dimensions. Details of the construction and performance are given.

*601,398*
**PB87-109484** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Experiences in Calibration of Neutron Survey Instruments.**
Final rept.,
R. B. Schwartz. Nov 85, 9p
Pub. in Proceedings of Workshop on Radiation Survey Instruments and Calibrations, Gaithersburg, MD., July 10-12, 1984, pF35-F43 1985.

Keywords: *Calibrating, *Remmeters, *Neutron dosimetry, Linearity.

It is shown that the measured calibration factors for many neutron remmeters vary considerably for nominally identical instruments, and even from one scale to another for the same instrument.

*601,399*
**PB87-117719** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Development of a 6 to 7 MeV Photon Field for Instrument Calibration.**
Final rept.,
K. C. Duvall, C. G. Soares, H. T. Heaton, and S. M. Seltzer. 1985, 4p
Pub. in Nuclear Instruments and Methods in Physics Research Section B-Beam Interactions WI 10-11, p942-945 May 85.

Keywords: Radiation protection, Calibrating, *Gamma sources, Thermoluminescent dosemeters, NaI detectors, MeV range 01-10, Response functions.

A photon source has been developed at the National Bureau of Standards to measure the response of radiological survey instruments to high-energy photons. The response of six commercial radiological survey instruments has been measured behind various thickness of plastic absorber. The results indicate that approximately 2.5 cm of plastic in front of these instruments is sufficient to discriminate against the associated high-energy electron contamination.

*601,400*
**PB87-122230** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Neutron Fluence and Cross Section Measurements for Fast Neutron Dosimetry.**
Final rept.,
G. P. Lamaze, D. M. Gilliam, E. D. McGarry, and A. Fabry. 1985, 9p
Pub. in Proceedings of International Conference on Nuclear Methods in Environmental and Energy Research (5th), Mayaguez, Puerto Rico, April 2-6, 1984, p293-601 1985.

Keywords: *Fast neutrons, Neutron cross sections, Fission neutrons, *Neutron dosimetry, Neutron fluence.

The National Bureau of Standards maintains three standard fields for fast neutron dosimetry calibrations: a (252)Cf fission spectrum, a (235)U fission spectrum, and an Intermediate Energy Standard Neutron Field (ISNF). The paper describes the fields and techniques that maintain the traceability of their fluence rates to NBS-I, the international standard radium-beryllium photoneutron source.

*601,401*
**PB87-122792** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**NBS (National Bureau of Standards) Facilities for the Study of Radiation-Protection Instruments.**
Final rept.,
M. Ehrlich, J. M. Selby, K. L. Swinth, E. J. Vallario, and B. L. Murphy. 1985, 22p
Pub. in Proceedings of Workshop on Radiation Survey Instruments and Calibration, Gaithersburg, MD., July 10, 1984, pF.13-F.34 Nov 85.

Keywords: *Radiation measuring instruments, *Radiation protection, Beta particles, Bremsstrahlung, Electron beams, Gamma rays, Radiation doses, US NBS.

An account is given of the NBS radiation facilities available for the study of radiation protection instruments. Covered are: The customary bremsstrahlung, cobalt-60, and cesium-137 beams; the new 6- to 7-MeV, essentially monoenergetic photon beam produced by (19)F(p, alpha gamma)(16)O reaction in the positive-ion Van de Graaff accelerator; the beta-particle beams (prometheum-137, thallium-204, and strontium-90 + yttrium-90); the essentially monoenergetic electron beams covering the energy range from about 0.2 to 2.5 MeV, produced in the electrostatic accelerator and the electron Van de Graaff accelerator; and the facility simulating a semi-infinite cloud containing a noble-gas radionuclide. The characterization of the facilities in terms of exposure rate or absorbed-dose rate to water at the point of instrument calibration and in terms of spectral distributions are described. Finally, examples are given of the result of studies of instruments in these radiation facilities.

*601,402*
**PB87-131835** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Accurate Determination of Gamma-Ray Energies for E < or = 2 MeV.**
Final rept.,
E. G. Kessler, G. L. Greene, R. D. Deslattes, and H. G. Boerner. 1985, 4p
Pub. in AIP (American Institute of Physics) Conference Proceedings 125, p921-924 1985.

Keywords: Fundamental constants, Reprints, *Gamma radiation, MeV range 01-10, Neutron mass.

A flat crystal spectrometer facility has been established at the 57 MW reactor at the Institut Laue-Langevin (ILL). The high flux reactor with the associated source changing facilities produces the intense capture gamma-rays needed for the high-resolution low-efficiency spectrometer. Initial measurements of gamma-ray energies up to 2 MeV from the reaction (35)Cl(n, gamma) have clearly demonstrated that sub-ppm measurements of intense sources are possible in the 2 to 4 MeV region. Energy values for the 517, 786, 788, 1165, 1951, 1959 keV lines are available with uncertainties of about 1 ppm. Three of these lines (786 + 1165 = 1951) satisfy the sum rule to better than 1 ppm. Future prospects for high energy capture gamma-ray measurements which impact on the neutron mass and the fundamental constants are briefly discussed.

## Radiation Shielding, Protection, & Safety

*601,403*
**DE85005518** PC **A02**/MF **A01**
National Bureau of Standards (NML), Washington, DC. Molecular Spectroscopy Div.
**Monte Carlo Calculation of Energy Deposition and Ionization Yield for High Energy Protons.**
W. E. Wilson, J. C. McDonald, J. J. Coyne, and H. G. Paretzke. Sep 84, 10p PNL-SA-12071, CONF-8409161-4
Contract AC06-76RL01830
Symposium on neutron dosimetry, Munich, F.R. Germany, 17 Sep 1984.

Keywords: *Neutron Transport, *Protons, *Tissue-Equivalent Materials, Charged-Particle Transport, Computer Calculations, Energy Losses, Ionization, MeV Range 01-10, MeV Range 10-100, Monte Carlo Method, Radiation Doses, Recoils, ERDA/654003, ERDA/654001.

Recent calculations of event size spectra for neutrons use a continuous slowing down approximation model for the energy losses experienced by secondary charged particles (protons and alphas) and thus do not allow for straggling effects. Discrepancies between the calculations and experimental measurements are thought to be, in part, due to the neglect of straggling. A tractable way of including stochastics in radiation transport calculations is via the Monte Carlo method and a number of efforts directed toward simulating positive ion track structure have been initiated employing this technique. Recent results obtained with our updated and extended MOCA code for charged particle track structure (3) are presented here. Major emphasis has been on calculating energy deposition and ionization yield spectra for recoil proton crossers since they are the most prevalent event type at high energies (>99% at 14 MeV) for small volumes. Neutron event-size spectra can be obtained from them by numerical summing and folding techniques. Data for ionization yield spectra are presented for simulated recoil protons up to 20 MeV in sites of diameters 2 to 1000 nm. 10 references. (ERA citation 10:011901)

*601,404*
**LA-UR-79-2685** MF **A01**
Los Alamos Scientific Lab., NM.
**Dosimetry Results for Big Ten and Related Benchmarks.**
G. E. Hansen, D. M. Gilliam, and J. A. Grunde. 1979, 10p CONF-791051-5
Contract W-7405-ENG-36
Pub. in Proceedings ASTM-EURATOM symposium on reactor dosimetry (3rd), Ispra, Italy, 1 Oct 1979.
Microfiche copies only.

Keywords: *Big ten reactor, Boron 10, Cross sections, Dosimetry, Flux density, Inelastic scattering, Lithium 6, Neutron flux, Nuclear reactions, Plutonium 239, Reaction kinetics, Uranium 233, Uranium 235, ERDA/654003.

Measured average reaction cross sections for the Big Ten central flux spectrum are given together with calculated values based on the US Evaluated Nuclear Data File ENDF/B-IV. Central reactivity coefficients for exp 233 U, exp 235 U, exp 239 Pu, exp 6 Li, and exp 10 B are given to check consistency of bias between measured and calculated reaction cross sections for these isotopes. Spectral indexes for the Los Alamos exp 233 U, exp 235 U, and exp 239 Pu metal critical assemblies are updated, utilizing the Big Ten measurements and interassembly calibrations, and their implications for inelastic scattering are reiterated. (ERA citation 05:005123)

*601,405*
**NUREG/CR-3628** PC **A05**/MF **A01**
Brookhaven National Lab., Upton, NY.

**Probability Based Safety Checking of Nuclear Plant Structures,**
B. Ellingwood. May 84, 85p BNL-NUREG-51737
Contract DE-AC02-76CH00016
Prepared in cooperation with National Bureau of Standards, Washington, DC. National Engineering Lab.

Keywords: *Nuclear power plants, *Structures, Design criteria, Safety, Loads(Forces), Reinforced concrete, Structural engineering, Probability.

This report describes the basis for the development of practical probability-based design criteria for nuclear plant structures. A brief critical review of existing criteria is provided to highlight desirable features of probability based-safety checking. A specific deterministic design criteria format is then recommended. Finally, the selection of a set of structures to test the validity of the probability-based checking equations is described. Statistical data on structural loads are summarized in an appendix.

*601,406*
**NUREG/CR-3876** PC **A05**/MF **A01**
Brookhaven National Lab., Upton, NY.
**Probability Based Load Combination Criteria for Design of Concrete Containment Structures,**
H. Hwang, S. Kagami, M. Reich, B. Ellingwood, and M. Shinozuka. Aug 85, 99p BNL-NUREG-51795
Contract DE-AC02-76CH00016
Prepared in cooperation with National Bureau of Standards, Gaithersburg, MD., and Columbia Univ., New York. Dept. of Civil Engineering and Engineering Mechanics.

Keywords: *Concrete structures, Design criteria, Reliability, Loads(Forces), *Containment buildings, *Earthquake engineering, Probability.

The report describes a research effort for the development of the probability-based load combination criteria for design of concrete containment structures. The proposed criteria are in a load and resistance factor design (LRFD) format. In order to test the performance objectives of the proposed criteria, four representative structures are selected using a Latin hypercube sampling technique. Next, the reliability analysis method developed by Brookhaven National Laboratory is employed to assess the reliability of these representative containments. The load factors for accident pressure due to the design basis accident and safe shutdown earthquake are derived for three target limit state probabilities. Other load factors are also discussed on the basis of prior experience with probability-based design criteria for ordinary building construction.

*601,407*
**PB86-195542** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Probability-Based Load Combinations for the Design of Concrete Containments.**
Final rept.,
H. Hwang, S. Kagami, M. Reich, B. Ellingwood, and M. Shinozuka. 1985, 13p
Sponsored by Brookhaven National Lab., Upton, NY.
Pub. in Nuclear Engineering and Design 86, n3 p327-339 1985.

Keywords: *Nuclear power plants, *Structural engineering, Loads(Forces), Reinforced concrete, Prestressed concrete, Probability theory, Reliability, Criteria, Reprints, Containment buildings.

The paper describes a procedure for developing probability-based load combinations for the design of concrete containments. The proposed criteria are in a load and resistance factor design (LRFD) format. The load factors and resistance factors are, in general, derived for use in limit states design and are based on target limit state probability. In the paper, the load factors for accident pressure due to the design basis accident and safe shutdown earthquake are derived for three target limit state probabilities. Other load factors are recommended on the basis of prior experience with probability-based design criteria for ordinary building construction.

*601,408*
**PB86-195989** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
**Probabilistic Descriptions of Resistance of Safety-Related Structures in Nuclear-Plants.**
Final rept.,
B. Ellingwood, and H. Hwang. 1985, 10p
Sponsored by Brookhaven National Lab., Upton, NY.
Pub. in Nuclear Engineering and Design 88, n2 p169-178 1985.

Keywords: *Nuclear power plants, *Structural engineering, Design, Reliability, Steels, Reinforced concrete, Fragility, Probability theory, Probability distribution functions, Reprints, Containment.

Calculations of reliability of safety-related nuclear plant structures require a knowledge of the probability distributions that describe their resistance. The study considers the applicability of existing statistical data for describing the resistance of steel and reinforced concrete nuclear plant structures. Probability distributions are recommended which can be used in assessing the reliability of containments and Category I structures, developing fragilities, and selecting appropriate resistance criteria for probability-based structural design.

*601,409*
**PB87-105268** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Recent Improvements In Neutron Energy Deposition Calculations.**
Final rept.,
R. S. Caswell, J. J. Coyne, and H. M. Gerstenberg. 1985, 9p
Pub. in Commission of the European Communities Report EUR 9762, Radiation Protection, v1 p255-263 1985.

Keywords: *Dosimetry, Monte Carlo method, Radiation protection, Reprints, *Neutron energy, *Neutron dosimetry, Computer applications.

At higher neutron energies calculations using the analytic method yield microdosimetric spectra in which the proton peak is narrower and shifted in peak energy when compared to experiment. The difference is usually attributed to the neglect of straggling in the calculation. In order to extend the calculational capability to this situation, the authors have written a Monte Carlo neutron energy deposition code which includes straggling of the energy depositions by charged particles in the sensitive volume. As a first consistency check, Monte Carlo calculations without straggling have been compared with the analytic method, and found to agree within the statistics of the Monte Carlo program. For 'thin' sensitive volumes for which the Landau distribution should be appropriate, the authors are using the Monte Carlo code to calculate lineal energy (y) distributions with proton straggling included for energies up to 15 MeV.

## Radioactive Wastes & Radioactivity

*601,410*
**PB87-132718** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
**Investigation of a Precise Static Leach Test for the Testing of Simulated Nuclear Waste Materials.**
Final rept.,
H. M. Kingston, D. J. Cronin, and M. S. Epstein. 1984, 13p
Pub. in Nuclear and Chemical Waste Management 5, n1 p3-15 1984.

Keywords: *Radioactive wastes, Chemical analysis, Precision, Concentration(Composition), Zinc, Calcium, Barium, Cesium, Molybdenum, Sodium, Silicon, Strontium, Reprints, *Leach tests.

The overall precision of the static leach test is determined by the summation of random effects caused by; (1) variance in the experimental conditions of the leaching procedure, (2) in homogeneity of the material to be leached, (3) variance of the analytical techniques used to determine elemental concentrations in the leachate. In the study, strict control of key experimental parameters was employed to reduce the source of variance. In addition, special attention to preparation of glass samples to be tested assured a high degree of homogeneity. Described here are the details of the reduction of these two sources of variance to a point where the overall test precision is limited by that of the analysis step. Of the elements determined B, Ba, Ca, Cs, Mo, Na, Si, Sr, and Zn; only Ca and Zn exhibited replicate imprecision significantly greater than that observed in the analysis of the leachate solutions.

## Reactor Materials

*601,411*
**PB86-185253** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Texture of Extruded Uranium Alloy by Neutron Diffraction.**
Final rept.,
C. S. Choi, and H. J. Prask. 1985, 6p
Pub. in Jnl. of Applied Crystallography 18, p413-418 1985.

Keywords: *Uranium alloys, *Nuclear reactor materials, Extrusions, Texture, Neutron diffraction, Tungsten, Fibers, Reprints.

The pole-density distributions of two hydrostatically extruded samples, a U-075 wt % Ti alloy and a U-075 wt % Ti/W composite alloy, were studied by neutron diffraction methods. Analysis of U 112, U 131 and U 111 pole figures revealed that the U phases of both samples posses a (010)/(340) duplex fiber texture with a probability ratio of approximately 2.8:1 in favor of the (010) direction. The W phase of the composite sample had a (110) fiber texture. The orientation distribution profiles of the fiber axes obtained from the rocking curves (as a function of the tilt angle) were represented best by a Gaussian-Lorentzian combination function. The full widths at half maximum of the distributions were approximately 21, 11, and 5 degs for the U (010), U(340) and W (110) fiber axes, rspectively.

## Reactor Physics

*601,412*
**HEDL-SA-1939-FP** PC **A02**/MF **A01**
National Bureau of Standards, Washington, DC.
**Double Fission Chamber for Absolute Fission Rate Measurements in Power Reactor Environments.**
J. L. Fuller, D. M. Gilliam, and J. A. Grundl. Aug 79, 9p CONF-791051-15
Contract EY-76-C-14-2170
Pub. in Proceedings ASTM-EURATOM symposium on reactor dosimetry (3rd), Ispra, Italy, 1 Oct 1979.
P

Keywords: *Fission chambers, *Fission fragment detection, Design, Diagrams, Fabrication, Performance, Testing, ERDA/360101.

A prototype fission chamber was tested and several chambers were built. The design and performance characteristics are presented. (ERA citation 05:008832)

*601,413*
**PB86-210036** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Observations of Spin Dependence In Superelastic Scattering of Polarized Electrons from Na(3P).**
Final rept.,
J. J. McClelland, M. H. Kelley, and R. J. Celotta. 1986, 6p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Electronic and Atomic Collisions, p239-244 1986.

Keywords: *Electron scattering, Reprints, *Atomic angular momentum, Superelastic scattering, *Exchange scattering.

Measurements are presented of spin asymmetries observed in the superelastic scattering of 10 eV electrons from laser excited Na(3P). Asymmetries as large as 16% are seen, despite the fact that the target is not spin-polarized. Data are presented both as a function of scattering angle and laser polarization angle. An interpretation of the effect is given in qualitative terms.

# OCEAN TECHNOLOGY & ENGINEERING

## Marine Engineering

*601,414*
**PB86-193398** PC **A04**/MF **A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Ductile Tearing Stability Analysis of a Ship Structure Containing a Crack Arrester Strake.**
Final rept. Sep 84-Sep 85,
A. V. Clark, and D. T. Read. Jan 86, 52p NBSIR-85/3038
Sponsored by David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.

Keywords: *Ships, Tearing, Tear strength, Ductility, *Crack arrest.

An analysis is presented for a structure made up of a crack arrester plate embedded in a ship structure. The crack arrester material is specified by its crack arrest temperature, its strength, and its tearing modulus T sub mat. The remainder of the structure is characterized as a set of springs and lumped masses. A stability condition is derived which states that the load-displacement curve of the structure as a whole must increase monotonically. An approximate quasistatic stability criterion sets a minimum material tearing modulus value that depends on the structural stiffness. Higher stiffness promotes effective crack arrest. A calculation including dynamic effects requires forward integration of a set of differential equations describing the fracture process and the motion of the structure.

*601,415*
**PB87-114096** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Fire Growth in Combat Ships,**
J. A. Rockett. Sep 86, 38p NBSIR-86/3451
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.

Keywords: *Naval ships, *Fire safety, Ventilation, Exhaust systems, Smoke, Mass transfer, FIRMOD computer program.

Several enrichments to FIRMOD, the Navy's ship battle damage estimation computer program, are considered. Enrichments recommended for immediate consideration are exponentially growing fires, ingestion by one ventilation system of smoke issuing from other ventilation system exhausts, and smoke transport between spaces served by the same ventilation system. Areas where further experimental work is recommended before FIRMOD enrichments are considered include fires ventilated primarily from above and buoyant smoke transport up shafts and ladderways.

## General

*601,416*
**PB87-140141** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Fluid-Structure Interaction Effects for Offshore Structures.**
Final rept.,
A. S. Veletsos, A. M. Prasad, and G. Hahn. Dec 86, 56p NBS/GCR-86/519
Prepared in cooperation with Rice Univ., Houston, TX. Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Offshore structures, Hydrodynamics, Structural engineering, Models, Dynamic response, Damping, Water waves, *Fluid-solid interactions, Morison equation.

Comprehensive analyses are made of the differences in the responses of simple models of offshore structures computed by the standard and extended versions of Morison's equation for the hydrodynamic forces, and of the effects and relative importance of the numerous parameters involved. The responses also are evaluated by the equivalent linearization technique and Penzien's decoupling technique, and the interrelationship and accuracy of these approaches are elucidated. The results are displayed graphically in the form of response spectra for absolute maximum displacement employing dimensionless parameters that are easy to interpret and use. In addition, the decoupling technique is generalized to include consideration of a current of constant velocity, and a simple modification is proposed which improves the accuracy of this approach. A particularly simple approximation is included for the hydrodynamic modal dampling values of multi-degree-of-freedom, stick-like systems.

# ORDNANCE

## Ammunition, Explosives, & Pyrotechnics

*601,417*
**PB87-145058** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Statistical Characterization of Electroexplosive Devices Relevant to Electromagnetic Compatibility Assessment.**
Technical note,
D. S. Friday, and J. W. Adams. May 86, 57p NBS/TN-1094
Also available from Supt. of Docs as SN003-003-02744-8. Sponsored by Army Aviation Systems Command, St. Louis, MO.

Keywords: *Initiators(Explosives), Electromagnetic compatibility, Electromagnetic pulses, Thermodynamic properties, Firing tests(Ordnance), Firing likelihood plots.

Electroexplosive devices (EEDs) are electrically fired explosive initiators used in a wide variety of applications. The nature of most of these applications requires that the devices function with near certainty when required and remain inactive otherwise. Recent concern with pulsed electromagnetic interference (EMI) and nuclear electromagnetic pulse (EMP) made apparent the lack of methodology for assessing EED vulnerability. A new and rigorous approach for characterizing EED firing levels is developed in the context of statistical linear models and is demonstrated in the paper. The authors combine statistical theory and methodology with thermodynamic modeling to determine the probability that an EED, of a particular type, fires when excited by a pulse of a given width and amplitude. The results can be applied to any type of EED for which the hot-wire explosive binder does not melt below the firing temperature. Included are methods for assessing model validity and for obtaining probability plots, called 'Firing Likelihood Plots'. A method of measuring the thermal time constant of an EED is given. This parameter is necessary to evaluate the effect of a train of pulses.

## Armor

*601,418*
**PB87-105524** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Law Enforcement Standards Lab.
**Ballistic Tests of Used Soft Body Armor,**
D. E. Frank. Sep 86, 44p NBSIR-86/3444
Sponsored by National Inst. of Justice, Washington, DC.

Keywords: *Body armor, Ballistics, Tests.

A sample of 24 ballistic resistant undergarments (soft body armor) from a production lot of 1500 originally distributed to 15 police departments throughout the United States in 1975 for issue to officers as part of a Law Enforcement Assistance Administration demonstration project, was tested for V50 ballistic limit. The program was a joint effort of the U.S. Department of Justice National Institute of Justice and the National Research Council of Canada Public Safety Project Office. Tests of ballistic limit were conducted on virgin armor that were never issued, and armor showing evidence of light, moderate, and heavy wear both dry and while wet. The results show that armor does not lose ballistic efficiency as a consequence of age.

## Guns

*601,419*
**AD-A130 809/7** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**Nonlinear Inverse Heat Transfer Calculations in Gun Barrels.**
Interim rept. 15 Jul 82-15 Jul 83,
Alfred S. Carasso. 15 Jul 83, 30p ARO-19643.1-MA
Contract MIPR-ARO-63-82
Pub. in Proceedings Trans Army Applied Math Comp. Conference (First), Washington, DC. May 1983.

Keywords: *Nonlinear analysis, *Heat transfer, *Gun barrels, *Interior ballistics, Conduction(Heat transfer), Thermocouples, Temperature, Measurement, Diffusion, Partial differential equations, Algorithms, Numerical analysis, Boundary value problems, Problem solving, Frequency, Time intervals, Cannons.

We consider the problem of determining the temperature history inside a gun barrel from embedded thermocouple measurements at some distance away from the inside wall. This inverse problem leads to an improperly posed initial value problem for a nonlinear system of partial differential equations, whenever the thermal properties are temperature dependent. We discuss a step-by-step marching algorithm for the numerical computation of such problems. The scheme is stabilized by appropriately filtering in the frequency domain at each step. We illustrate this technique with a numerical experiment on a nonlinear problem whose exact solution is known. The basic ideas are applicable to other unstable evolution equations.

# PHOTOGRAPHY & RECORDING DEVICES

## Recording Devices

*601,420*
**PB86-209301** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Transient Response Characterization of Waveform Recorders.**
Final rept.,
T. M. Souders, D. R. Flach, and H. K. Schoenwetter. 1985, 4p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Pulsed Power Conference (5th), Arlington, VA., June 10-12, 1985, p352-355.

Keywords: *Waveforms, *Recording instruments, Transient response, Tests.

Test methods for characterizing the transient response of waveform recorders are presented, together with typical test results. The methods, based on the use of a precision, programmable step generator developed at NBS, are suitable for recorders having up to 10 bits of resolution and 100 MHz bandwidth.

# PHYSICS

## Acoustics

*601,421*
**AD-A148 921/0** PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.
**Acoustic Emission Transducer Calibration by Means of the Seismic Surface Pulse.**
Technical rept.,
F. R. Breckenridge. Apr 82, 9p Rept no. TR-82-1
Contracts N00014-81-F-0009, N00014-82-F-0004
Also Pub. in Jnl. of Acoustic Emission, v1 n2 p87-94 Apr 82.

Keywords: *Transducers, *Calibration, *Acoustic emissions, Elastic waves, Voltage, Output, Error analysis, Naval research.

A system for calibrating transducers as receivers of elastic waves at the surface of a solid medium has been developed and is now in use at the National Bureau of Standards (NBS). The method provides the voltage output of the transducer when mounted on a surface whose motion is known. The measurement is made over the range of 100 kHz to 1 MHz and is designed with the calibration of acoustic emission (AE) transducers in mind. An error analysis is given.

*601,422*
**PB86-185303** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Gas-Filled Spherical Resonators: Theory and Experiment.**
Final rept.,
M. R. Moldover, J. B. Mehl, and M. Greenspan. Feb 86, 18p
Pub. in Jnl. of the Acoustical Society of America 79, n2 p253-270 Feb 86.

Keywords: *Acoustic resonators, Acoustic velocity, Argon, Thermodynamic properties, Reprints.

Gas-filled spherical resonators are excellent tools for routine measurement of thermophysical properties. The radially symmetric gas resonances are nondegenerate and have high Q's (typically 2000-10,000). Thus they can be used with very simple instrumentation to measure the speed of sound in a gas with an accuracy of 0.02%. The authors have made a detailed study of a prototype resonator filled with argon (0.1-1.0 MPa) at 300 K, with the objective of discovering those phenomena which must be understood to use gas-filled spherical resonators to measure the thermodynamic temperature and the universal gas constant R. The resonance frequencies f(N) and half-widths g(N) were measured for nine radially symmetric modes and nine triply-degenerate nonradial modes with a precision near 10 to the -7th power f(N). The data were used to develop and test theoretical models for the geometrically simple oscillating system.

*601,423*
**PB86-188471** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Transient Waves in an Elastic Plate: Theory and Experiment Compared.**
Final rept.,
T. M. Proctor, F. R. Breckenridge, and Y. H. Pao. 1983, 3p
Pub. in Jnl. of the Acoustical Society of America 74, n6 p1905-1907 1983.

Keywords: *Waveforms, Detectors, Transducers, Reprints, *Acoustic emissions.

Waveforms calculated by generalized ray theory for a thick plate driven by a step-function point force are compared with experimental waveforms obtained on a glass plate using an improved piezoelectric displacement-sensing transducer.

*601,424*
**PB86-239969** PC A08/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Electrical Performance Tests for Audio Distortion Analyzers.**
Final rept.,
O. B. Laug, G. N. Stenbakken, and T. F. Leedy. Jan 86, 161p NBS/TN-1219
Sponsored by Army Communications-Electronics Command, Fort Monmouth, NJ.

Keywords: *Sound analyzers, Performance tests, Distortion, Computer programs.

Electrical performance test procedures for audio distortion analyzers were developed by the National Bureau of Standards for the U.S. Army Communications-Electronics Command. The report provides detailed, step-by-step test procedures that are based on specifications supplied by the Army for purposes of evaluating audio distortion analyzer bid samples. Examples of data sheets and tables are also provided for recording interim and final results. The report discusses the philosophy of each measurement procedure with a view toward providing an understanding of the basic metrology required to perform the measurements. In addition, the sources of measurement error are discussed. The primary applications and basic principles of modern audio distortion analyzers are also presented.

*601,425*
**PB87-110086** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
**Uncertainties in the Cross-Spectral Method for Acoustic Intensity under Semireverberant Conditions.**
Final rept.,
M. Villot, T. W. Bartel, and S. L. Yaniv. 1986, 11p
Pub. in Jnl. of the Acoustical Society of America 79, n3 p691-701 Mar 86.

Keywords: *Acoustic measurement, Intensity, Reprints.

Measurements were performed, under semireverberant conditions, to examine uncertainties in the two-microphone cross-spectral method for determining acoustic intensity. Calculations of the pressure gradient error, the error associated with the correction for phase mismatch, and the cross-spectrum random error are discussed. The results of preliminary tests performed under free-field and plane-wave conditions are also presented. The influence of semireverberant conditions on the accuracy of the intensity measurement was studied through the use of a standing-wave tube as a reference sound source. With the tube source placed in a 112-cu m room having reverberation times of about 0.5 s, the radiated power was determined both from the intensity measured inside the tube and from the intensity integrated over a spherical surface enclosing the source.

*601,426*
**PB87-134276** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Practical Sound-Reducing Enclosure for Laboratory Use.**
Final rept.,
D. Hils, J. E. Faller, and J. L. Hall. 1986, 3p
Pub. in Review of Scientific Instruments 57, n10 p2532-2534 Oct 86.

Keywords: *Acoustic absorption, *Enclosures, Laboratory equipment, Noise reduction, Design, Reprints, Acoustic attenuation.

The authors describe the design of a sound-reducing laboratory enclosure. The unit fits directly over the experiment and is hoisted to the ceiling during setup and adjustment stages. The advantages of the design are its modest cost, saving of space, and the fact that no door is required. The average sound isolation achieved is 30 dB, typical for a wall mass per unit area of 35 kg/sq m.

*601,427*
**PB87-134482** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
**Institute of Electrical and Electronics Engineers (IEEE) Ultrasonics Symposium.**
Final rept.,
G. V. Blessing. 1986, 3p
Pub. in Ultrasonics 24, n6 3p Nov 86.

Keywords: *Meetings, Reprints, *Ultrasonics.

The IEE 1985 Ultrasonics Symposium, a three-day international conference held in San Francisco 16-18 October of 1985, is reviewed here. The Conference covers the theory, development, and application of ultrasonic techniques and tools. Over one-third of the papers presented were from outside the United States. Symposium proceedings have been published and are available from the IEEE publishing headquarters in New Jersey.

## Fluid Mechanics

*601,428*
**PB86-160793** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysical Properties Div.
**Decay of Swirling Gas Flow in Long Pipes.**
Final rept.,
S. E. McManus, B. R. Bateman, J. A. Brennan, I. Vasquez, and D. Mann. 1985, 5p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in Proceedings of the American Gas Association Operating Section (1985), Boston, MA., May 20-22, 1985, p629-633.

Keywords: *Gas flow, *Flow measurement, Swirling, Decay, Pipe flow.

A characterization of swirling flow of nitrogen gas at ambient temperature, pressure of 4 MPa (600 psi), and Reynolds numbers of 800,000 to 1,400,000 is presented. Possible flowmeter measurement errors in a pipe of circular cross-section are given. An instrumented test section containing a hot wire anemometer and a directional pilot tube for the measurement of swirl angles and velocities are described. Results suggest that large values of swirl are possible in gaseous flow, that the decay of the swirl is very slow at high Reynolds numbers, and that reliance on long lengths of pipe to reduce swirl to acceptable levels may not be a practical solution to eliminating potential flow measurement errors attributable to swirl.

*601,429*
**PB86-187267** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**Double-Diffusive Convection with Sidewalls.**
Final rept.,
G. B. McFadden, S. R. Coriell, and R. F. Boisvert. Sep 85, 7p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Physics of Fluids 28, n9 p2716-2722 Sep 85.

Keywords: *Diffusivity, *Fluid flow, Convection, Stability, Reprints, Sidewalls.

The effect of rigid vertical boundaries on the onset of convective instability is calculated for the salt finger regime of double-diffusive convection. The unperturbed state is a quiescent fluid with constant vertical gradients of temperature and solute, which are stabilizing and destabilizing, respectively. The horizontal boundaries are taken to be stress-free and perfectly conducting. The lateral boundaries are perfectly insulating for solute. Changing from thermally insulating to thermally conducting sidewalls results in a strong destabilization of the flow for large thermal Rayleigh numbers even in the limit that the separation between the sidewalls approaches infinity. Further, for thermally conducting sidewalls, a decrease in the separation of the sidewalls may destabilize the system.

*601,430*
**PB86-187697** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Tagged Particle Fluctuations in Uniform Shear Flow.**
Final rept.,
M. C. Marchetti, and J. W. Dufty. 1983, 23p
Pub. in Jnl. of Statistical Physics 32, n2 p255-277 1983.

Keywords: *Boltzmann equation, *Shear flow, Kinetic theory, Nonequilibrium flow, Velocity, Reprints.

The nonlinear Boltzmann and Boltzmann-Lorentz equations are used to describe the dynamics of a tagged particle in an nonequilibrium gas. For the special case of Maxwell molecules with uniform shear flow, an exact set of equations for the average position and velocity, and their fluctuations, is obtained. The results apply for arbitrary magnitude of the shear rate and include the effects of viscous heating. A generalization of Onsager's assumption of the regression of fluctuations is found to apply for the relationship between the equations for the average dynamics and those for the time correlation functions. The connection between fluctuations and dissipation is described by the equations for the equal-time correlation function.

*601,431*
**PB86-196722** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
**Chemically Reacting Turbulent Flow.**
Final rept. 1 Oct 82-30 Sep 85,
W. M. Pitts, and T. Kashiwagi. Mar 86, 43p NBSIR-85/3299
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Turbulent flow, *Chemical reactions, Rayleigh scattering, Light scattering, Reynolds number, Flow visualization.

The report summarizes the results of the first three years of a study on chemically reacting turbulent flow. The development of new diagnostics for variable density flows are described. These include Rayleigh light scattering for real-time, spatially-resolved concentration measurements, combined Rayleigh light scattering and hot-wire anemometry for simultaneous concentration and velocity measurements, and the development of a digital line camera which has allowed the concentration measurements to be made along a line. A study of heat transfer from heated cylinders is discussed which has generated a much improved correlation of experimental results. These studies have also included a limited investigation of Reynolds number effects. The observed dependence of the mixing behavior on the density ratio and Re have led us to make new hypotheses concerning the nature of turbulent mixing.

*601,432*
**PB86-200375** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
**New Diagnostic Technique for Simultaneous, Time-Resolved Measurements of Concentration and Velocity in Simple Turbulent Flow Systems.**
Final rept.,
W. M. Pitts, B. J. McCaffrey, and T. Kashiwagi. 1983, 6p
Contract AFOSR-MIPR-83-00012
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Proceedings of the Symposium on Turbulent Shear Flows (4th), Karlsruhe, West Germany, September 12-14, 1983, p15.22-15.27.

Keywords: *Flow measurement, *Turbulent flow, Rayleigh scattering, Hot wire anemometers, Velocity measurement, Cross correlation.

A new experimental method is described which allows the simultaneous real-time measurement of concentration and velocity in simple flow fields of binary gas mixtures. This method combines the use of Rayleigh light scattering for concentration measurements and hot-wire (or hot-film) anemometry. Calibration methods and representative results are discussed.

*601,433*
**PB86-210234** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Measurement of Air Velocity Components of Natural Convective Interzonal Air Flow.**
Final rept.,
B. M. Mahajan. 1986, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Air Movement and Distribution Conference, Lafayette, IN., May 27-29, 1986, p95-103 May 86.

Keywords: *Air flow, Flow visualization, Convection, Doors.

Recent flow visualization tests performed at the National Bureau of Standards Passive Solar Test Facility, indicated that the natural convective interzonal flow through a doorway is three dimensional with the velocity components perpendicular to the plane of the opening and the plane of the floor appearing dominant. In order to further investigate the velocity components of the interzonal airflow through a doorway an experimental study was undertaken.

*601,434*
**PB86-210242** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Inter-room Air Flow by Natural Convection via a Doorway Opening.**
Final rept.,
B. M. Mahajan. 1986, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in ASME (American Society of Mechanical Engineers) Solar Energy Conference (SED 8th Annual), Anaheim, CA., April 13-16, 1986, p473-481.

Keywords: *Air flow, Doors, Convection, Temperature, Velocity.

The objectives of the study were to measure the temperature and velocity profiles of the air moving by natural convection through a doorway opening; and compare the measured data with the values predicted by the simple existing algorithms. Two types of experiments were carried out in two sets of full-size adjoining rooms of the NBS passive solar test facility.

*601,435*
**PB87-100244**
(Order as PB87-100186, PC **A08**/MF **A01**)
Brunel Univ., Uxbridge (England).
**Improvements in the Application of the Numerical Method of Characteristics to Predict Attenuation in Unsteady Partially Filled Pipe Flow,**
J. A. Swaffield, and K. Maxwell-Standing. Jun 86, 8p
Grant NANB-D-0510
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v91 n3 p149-156 May-Jun 86.

Keywords: *Pipe flow, *Unsteady flow, Pipes(Tubes), Interpolation, Attenuation, Iteration, Numerical solution, Method of chracteristics.

The use of linear interpolation and simplified iteration procedures are shown to introduce inaccuracies to the rectangular grid method of characteristics, particularly when applied to subcritical flows. Comparisons of experimental and computational results are presented illustrating the use of Everett and Newton-Gregory interpolation, in addition to a more complex iteration procedure, to substantially improve the method's ability to maintain both steady uniform flows under subcritical conditions, and retain wave steepness during propagation along the drainage pipe. The results presented will be directly applicable to the building drainage network model previously developed at Brunel University with the support of NBS CBT grant aid.

*601,436*
**PB87-106035** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Numerical Modeling of Vortex Merging in Axisymmetric Mixing Layers.**
Final rept.,
R. W. Davis, and E. F. Moore. 1985, 6p
Pub. in Lecture Notes in Physics 218, p180-185 1985.

Keywords: Two dimensional flow, Vortices, Stability, Jets, *Computational fluid dynamics, *Mixing layers.

The paper presents numerical solutions for spatially-developing axisymmetrix mixing layers. The vortex merging inside these mixing layers is driven by small perturbations derived from linear inviscid stability theory. It is found that, as seen experimentally in the two-dimensional case, the merging process is controlled by the frequency content of the forcing function. Thus it is possible to manipulate the downstream behavior of the mixing layer by altering the applied perturbation. Although the forced temporally-developing mixing layer with its simpler boundary conditions has been studied computationally, this is not as desirable as studying the spatially-developing case which occurs in most physical situations.

*601,437*
**PB87-106043** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
**Numerical Study of Vortex Merging in Mixing Layers.**
Final rept.,
R. W. Davis, and E. F. Moore. 1985, 10p
Pub. in Physics of Fluids 28, n6 p1626-1635 1985.

Keywords: Two dimensional flow, Unsteady flow, Vortices, Mixing, Reprints, *Computational fluid dynamics, *Mixing layers.

Numerical solutions are presented for forced spatially-developing axisymmetric and two-dimensional mixing layers. The numerical scheme employs quadratic upwind differencing for convection and a Leith-type of temporal differencing in order to solve the incompressible Navier-Stokes and continuity equations. The applied forcing function is derived from linear inviscid stability theory. The resulting large-scale vortex dynamics is visualized by means of streakline and isovorticity contour plots. It is seen that the vortex merging behavior in both types of mixing layers is determined by the subharmonics present in the forcing function. Manipulation of the vortex dynamics in a predictable fashion is possible through alterations in the frequency content of this applied forcing. Reynolds number is shown to be of only minor importance.

*601,438*
**PB87-109682** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.
**Non-Newtonian Flow between Concentric Cylinders and the Effects of Finite Compressibility.**
Final rept.,
J. C. Rainwater, and H. J. M. Hanley. Nov 85, 11p
Sponsored by Department of Energy, Washington, DC.
Pub. in International Jnl. of Thermophysics 6, n6 p595-605 Nov 85.

Keywords: *Compressibility, Thermophysical properties, Compressible flow, Reprints, *Non-Newtonian flow, Concentric cylinders, Weissenberg effect.

Previous studies of the flow of a model soft-sphere liquid between rotating vertical concentric cylinders have predicted an enhanced depression of the free surface at the inner cylinder and the necessity and importance of accounting for finite compressibility. In those studies the rheological properties of the liquids were taken directly from computer simulations, whereas in the present work the liquid properties are altered in a controlled manner and the fluid dynamics problems is again solved numerically and self-consistently with the original boundary conditions. Specific alterations include the removal of all non-Newtonian properties, the change in sign of a generalized viscosity to create a rodclimbing or Weissenberg effect, and the removal of shear dilatancy or increase in pressure with shear. The conclusion is that nonzero compressibility needs to be taken into account only in the presence of shear dilatancy.

*601,439*
**PB87-117735** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.
**Note on Flow Rate and Leak Rate Units.**
Final rept.,
C. D. Ehrlich. 1986, 2p
Pub. in Jnl. of Vacuum Science and Technology A 4, n5 p2384-2385 Sep/Oct 86.

Keywords: *Gas flow, *Leakage, Calibrating, Vacuum, Reprints.

The confusion in the literature and in the laboratory surrounding the terminology and units of gas flow rates, particularly as applied to calibrated leak artifacts, has prompted this discussion of leak rate units. Special attention is paid to conflicting usages of the term 'throughput,' and how this frequently leads to the loss of crucial information about the gas temperature and hence the true gas flow rate. The advantages of expressing leak rates in 'mol/s,' avoiding the complications of both the explicit mention of temperature in the unit and the need for agreement on 'standard' temperature and pressure, are also discussed.

*601,440*
**PB87-128328** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

## Fluid Mechanics

**Thermometer for Fast Response in Cryogenic Flow.**
Final rept.,
B. Louie, R. Radebaugh, and S. R. Early. 1986, 12p
Sponsored by Air Force Wright Aeronautical Labs., Wright-Patterson AFB, OH.
Pub. in Advances in Cryogenic Engineering 31, p1235-1246 1986.

Keywords: *Temperature measuring instruments, *Resistance thermometers, Silicon, Thin films, Sapphires, Substrates, Reprints, *Cryogenic fluids, Acoustic waves, Transients.

The measurement of transient temperatures in cryogenic fluid flow requires a highly sensitive, intrinsically fast sensor that is in good thermal contact with the fluid but in poor thermal contact with the solid walls confining the fluid. A resistance thermometer made from a 1 micrometer thick silicon layer on a 125 micrometers thick sapphire substrate has a calculated intrinsic response time of about 10 ns at 4 K, and its sensitivity is comparable to germanium or carbon thermometers in the range of 1 - 80 K. The paper describes a novel construction method to mount the small silicon-on-sapphire thermometer in an oscillating fluid flow.

*601,441*
**PB87-134383** PC **A16**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
**Investigation of Horizontal Flow Boiling of Pure and Mixed Refrigerants,**
H. D. Ross. Nov 86, 359p NBSIR-86/3450
Portions of this document are not fully legible. Sponsored by Department of Energy, Washington, DC.

Keywords: *Heat transfer, *Refrigerants, Two phase flow, Boiling, Fluid flow, Mixtures.

The research involved determining experimental heat transfer coefficients (HTC), examining the phenomena involved in the physical process, and analyzing the predictive ability of available models and correlations. This work was done for pure R152a and R13B1 and for mixtures of these refrigerants. The mixtures yielded sharply lower heat transfer coefficients than either pure refrigerant. With pure refrigerants full suppression of nucleate boiling (FSNB) occurs only at rather low pressures. Correlative evidence suggests that suppression is easier to achieve with mixtures than pure fluids. In the evaporation-dominated heat transfer regime, Chen's correlation was successfully applied to the refrigerants with and without the occurrence of FSNB conditions. In the nucleate boiling dominated regime, the Stephan and Abdelsalam method was validated for pure fluids, and used successfully with Thome's method for mixtures. Pressure drop correlations for pure fluids were also extended to mixtures without modification.

## Optics & Lasers

*601,442*
**PATENT-4 590 597** Not available NTIS
Department of Commerce, Washington, DC.
**Modulation Transfer Spectroscopy for Stabilizing Lasers.**
Patent,
M. Long-sheng, L. Hollberg, J. H. Shirley, and J. L. Hall. Filed 21 May 84, patented 20 May 86, 6p PB86-201985, PAT-APPL-6-612 291
Supersedes PB84-224641.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 $1.00.

Keywords: *Lasers, *Frequency stability, *Stabilization, *Patents, Gases, *Modulation transfer spectroscopy, Optical resonators, PAT-CL-372-32.

A method and apparatus are disclosed for precisely stabilizing a laser to a sub-Doppler resonance of an absorbing gas contained in a cell located external to the laser resonator. Stabilization is based on the detection of modulation transferred onto a previously unmodulated probe beam by the non-linear interactions of the absorbing gas located in a cell which is subject to a counter-running, frequency-modulated saturation beam. Alternatively, the further modulation of the saturation beam can be detected.

*601,443*
**PB86-160132** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Non-Resonant Laser-Driven Ionization of Condensing Vapors: A Mechanism Based on Cluster Fragmentation.**
Final rept.,
W. T. Hill. Jul 85, 6p
Sponsored by Research Corp., New York, and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Optics Communications 54, n5 p283-288, 1 Jul 85.

Keywords: *Barium, *Ionization, Argon, Vapors, Condensing, Reprints, Laser radiation.

Anomalous ionization has been observed following broad-band, nonresonant irradiation of an atomic barium vapor at high Ar buffer gas pressures. Time resolved hook measurements involving several neutral and ion states of Ba show that excited neutral and ion densities between 10 to the 14th power-10 to the 15th power/cc can be generated. The dependence of the densities on Ar pressure, time and Ba vapor density is suggestive of an ionization mechanism based on laser vaporization of barium droplets.

*601,444*
**PB86-160629** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Monochromatic Source of Lyman-alpha Radiation.**
Final rept.,
J. Z. Klose, J. M. Bridges, and W. R. Ott. 1985, 4p
Contract NA80RA-G-03527
Sponsored by National Oceanic and Atmospheric Administration, Rockville, MD.
Pub. in Applied Optics 24, n14 p2263-2266, 15 Jul 85.

Keywords: *Lyman alpha radiation, Far ultraviolet radiation, Monochromatic radiation, Standards, Radiometry, Reprints, *Light sources, Hydrogen atoms.

A source has been developed which produces a pure spectrum of Lyman-alpha radiation (1215.7A). The source incorporates a wavelength selective filter and an rf-excited helium-filled lamp containing a mixture of uranium and uranium hydride in a sidearm. The uranium serves as a getter to eliminate atmospheric contaminants, and the uranium hydride, when heated, supplies H2 in a reproducible manner. The filter consists of a flowing-oxygen cell and a narrowband interference filter. The distinctive advantage of the devices is that radiation in the VUV at a well-defined wavelength is obtained without the use of a monochromator. Characteristics of the source and measurements of the irradiance of the spectral line are given for a typical lamp. The irradiance and spectral purity are seen to be not strongly dependent on oxygen flow.

*601,445*
**PB86-161023** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Free-Space Propagation of Ultrashort Light Pulses.**
Final rept.,
J. Cooper, and E. Marx. 1985, 10p
Pub. in Jnl. of the Optical Society of America A 2, n10 p1711-1720 Oct 85.

Keywords: *Light pulses, Maxwells equations, Boundary value problems, Reprints.

A boundary-value problem for Maxwell's equations is formulated whose solutions represent ultrashort pulses of electromagnetic energy that travel along an axis. A paraxial approximation to the solution is introduced that in the case of Gaussian boundary data, is expressed as a single integral over frequency. Calculations are presented for a pulse of Gaussian cross section and Gaussian time profile. A careful study is made of the error introduced by the paraxial approximation, and an error bound is derived.

*601,446*
**PB86-163490** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Characterization of Aircraft-Collected Particles Present in the Arctic Aerosol: Alaskan Arctic, Spring 1983.**
Final rept.,
P. J. Sheridan, and I. H. Musselman. 1985, 8p
Sponsored by National Oceanic and Atmospheric Administration, Washington, DC., National Aeronautics and Space Administration, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in Atmospheric Environment 19, n12 p2159-2166 1985.

Keywords: *Electron microscopy, Particles, Reprints, *Artic aerosols, *Laser microprobe analysis.

Eight hundred submicrometer and 516 large and giant (> 1 micrometer) particles collected by cascade impactor from Artic haze aerosol were characterized using analytical electron microscopy. Selected particles were also analyzed using laser microprobe mass analysis. Over 97 percent of the analyzed submicrometer particles showed high sulfate concentrations, and a large majority (96 percent) of these appeared to have been collected directly as H2SO4 droplets. Anthropogenic particles, including graphitic carbon (soot), coal and oil fly ash, and Cu-Ni smelter emissions were observed in the coarser particle fraction. 'Air trajectories indicate much of the aerosol passed over industrialized regions in the U.S.S.R.

*601,447*
**PB86-164456** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Servo Control of Amplitude Modulation in FM Spectroscopy: Shot-Noise Limited Measurement of Water Vapor Pressure-Broadening.**
Final rept.,
N. C. Wong, and J. L. Hall. 1985, 2p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Proceedings of International Conference on Laser Spectroscopy (7th), Maui, HI., June 24-28, 1985, p393-394.

Keywords: Amplitude modulation, Phase modulation, Laser beams, Sensitivity, Servomechanisms, Water vapor, *Frequency modulation spectroscopy, *Laser spectroscopy.

The authors have developed and demonstrated an active servo system to suppress the AM noise of a phase modulated laser beam to achieve shot-noise limited detection in a linear absorption experiment.

*601,448*
**PB86-164464** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Servo Control of Amplitude Modulation in Frequency-Modulation Spectroscopy: Demonstration of Shot-Noise-Limited Detection.**
Final rept.,
N. C. Wong, and J. L. Hall. 1985, 7p
Contract N00014-77-C-0656, Grant NSF-PHY82-00805
Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in Jnl. of the Optical Society of America B2, n9 p1527-1533 Sep 85.

Keywords: Laser beams, Amplitude modulation, Phase modulation, Sensitivity, Iodine, Electrooptics, Servomechanisms, Reprints, *Frequency modulation spectroscopy, *Laser spectroscopy.

The authors describe and demonstrate a new method to reduce actively the amplitude modulation of a phase-modulated laser to the shot-noise limit. This theoretical limit of ultrahigh sensitivity of FM spectroscopy is achieved in a linear absorption experiment with iodine.

*601,449*
**PB86-168259** PC **A25**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Laser Induced Damage in Optical Materials: 1983.**
Final rept.,
H. E. Bennett, A. H. Guenther, D. Milam, and B. E. Newnam. Nov 85, 583p NBS/SP-688
See also PB84-175124. Proceedings of a symposium held at Boulder, Colorado, November 14-16, 1983. Also available from Supt. of Docs as SN003-003-

02706-5. Library of Congress catalog card no. 85-600630. Sponsored by American Society for Testing and Materials, Philadelphia, PA., Office of Naval Research, Arlington, VA., Department of Energy, Washington, DC., and Defense Advanced Research Projects

Keywords: *Optical materials, *Meetings, Laser materials, Lasers, Damage, Thin films, Surfaces, Mirrors.

The Symposium was divided into sessions concerning Materials and Measurements, Mirrors and Surfaces, Thin Films, and finally Fundamental Mechanisms. As in previous years, the emphasis of the papers presented at the Symposium was directed toward new frontiers and new developments. Particular emphasis was given to materials for high power apparatus. The wavelength range of prime interest was from 0.6 micrometers to the uv region. Highlights included surface characterization, thin film-substrate boundaries, and advances in fundamental laser-matter threshold interactions and mechanisms. The scaling of damage thresholds with pulse duration, focal area, and wavelength was discussed in detail.

*601,450*
**PB86-182367** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Documentation of the NBS APD (National Bureau of Standards Avalanche) and PIN Calibration Systems for Measuring Peak Power and Energy of Low-Level 1.064 Micrometer Laser Pulses,**
A. L. Rasmussen, and A. A. Sanders. Dec 85, 75p
NBSIR-85/3032
Errata sheet inserted. Sponsored by Aerospace Guidance and Metrology Center, Newark AFS, OH., and Naval Plant Representative, Pomona, CA. Metrology Engineering Center.

Keywords: *Power measurement, *Photodiodes, *Standards, Light pulses, Near infrared radiation, Infrared lasers, Maintenance, Energy, Continuous radiation, *Transfer standards, *Laser radiation, *Calibration, PIN diodes, Beam splitters.

National Bureau of Standards APD (avalanche) and PIN silicon photodiode transfer standards are documented for a calibration service to measure 1.064 micrometer laser pulses from about 10 to the -8th power to about 10 to the -4th power W peak power and about 10 to the -16th power to about 10 to the -11th power J energy. A modulated cw measurement system generating known low-level pulses is described. Calibration support equipment, systematic and random errors, and computer programs and calibration data are also described.

*601,451*
**PB86-185329** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
**Strength and Fatigue Properties of Optical Glass Fibers Containing Microindentation Flaws.**
Final rept.,
T. P. Dabbs, and B. R. Lawn. Nov 85, 7p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of the American Ceramic Society 68, n11 p563-569 Nov 85.

Keywords: *Fiber optics, Fatigue(Materials), Strength, Reprints, *Optical fibers, Lifetime.

The inert strength and dynamic fatigue properties of fused-silica optical fibers are studied using subthreshold indentation flaws, i.e., flaws without radial cracks. Direct observations of the indentation sites up to the point of failure indicate that the property differences can be interpreted in terms of a transition from propagation-controlled to initiation-controlled fracture instabilities at reduced contact loads. The subthreshold instability condition is modeled qualitatively as a two-step, deformation-fracture process, with strong emphasis on the importance of residual stress fields in parametric evaluations. The relevance of the results to the practical issue of fiber reliability, most notably in connection with the potential dangers of using macroscopic crack velocity data to predict long-lifetime characteristics, is addressed.

*601,452*
**PB86-186673** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**New Far Infrared Laser Lines Obtained by Optically Pumping (13)CD3OD.**
Final rept.,
E. C. C. Vasconcellos, and K. M. Evenson. 1985, 11p
Grant NSF-INT80-19014
Sponsored by National Science Foundation, Washington, DC., and Conselho Nacional de Pesquisas, Rio de Janeiro (Brazil).
Pub. in International Jnl. of Infrared and Millimeter Waves 6, n11 p1157-1167 1985.

Keywords: *Infrared lasers, Far infrared radiation, Carbon dioxide lasers, Reprints, *Methyl alcohol lasers, Carbon 13.

Laser action was obtained in 34 far infrared lines for the first time in fully deuterated methyl alcohol with the (13)C isotope (13)CD3OD). The frequency of 13 lines was measured. The molecule was pumped by cw CO2 laser. The wavelength, the relative polarization, the relative intensity of most lines, the frequency, and the CO2 pump frequency offset of the strongest lines were measured. The new lines are distributed in the wavelength region from 75.27 micrometers to 464.7 micrometers.

*601,453*
**PB86-187143** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Absolute Physical Quantities.
**Longitudinal Ramsey Fringe Spectroscopy in an Atomic Beam.**
Final rept.,
J. J. Snyder, J. Helmcke, D. Zevgolis, and M. Glaeser. 1983, 5p
Pub. in Springer Series in Optical Sciences 40, n6 p108-112 1983.

Keywords: *Frequency standards, Atomic spectroscopy, Calcium, Reprints, Laser spectroscopy, Line broadening.

For ultra-high resolution spectroscopy such as optical frequency standards, the value of thermal sources such as atomic beams is currently limited by second-order Doppler broadening. The use of a longitudinal interaction geometry in which an atomic beam crosses the counter-propagating laser fields at a shallow angle is able to reduce second-order Doppler broadening to an insignificant level as well as to provide long interaction times without the necessity of large diameter optical beams. The authors have analyzed the geometry for the case of the long-lived calcium intercombination line, and conclude that when combined with pulsed (Ramsey) excitation, the longitudinal interaction geometry could be used with a thermal calcium beam to create an optical frequency standard with a reproducibility of the order of 10 to the -14th power for a few seconds of averaging time. Their initial experimental results have demonstrated the first use of the longitudinal geometry.

*601,454*
**PB86-193919** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Spectrophotometric Tests Using a Dye-Laser-Based Radiometric Characterization Facility.**
Final rept.,
A. R. Schaefer, and K. L. Eckerle. 1984, 7p
Pub. in Applied Optics 23, n2 p250-256 1984.

Keywords: *Spectrophotometry, *Radiometry, Optical filters, Optical detection, Reprints, Laser applications, Dye lasers, Spectral response.

A new high accuracy dye laser based system useful for measuring the spectral transmittance of filters or the spectral response of optical detectors has recently been developed at NBS. The paper describes the system and discusses the results of measurements made for purposes of comparison with a high accuracy spectrophotometer, also developed at NBS.

*601,455*
**PB86-202405** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Noise and Fluctuations in Multiphoton Processes.**
Final rept.,
P. Zoller. 1984, 11p
Pub. in Proceedings of the Rochester Conference on Coherence and Quantum Optics (5th), Rochester, NY., June 13-15, 1983, p383-393 1984.

Keywords: Light transmission, Stark effect, Stochastic processes, Noise, *Multi-photon processes, Laser radiation.

Aspects of how to formulate and solve the problem of resonant multiphoton processes in stochastic fields are summerized, emphasizing the connection with the (quantum) theory of laser coherence. Some recent results are discussed including Stark shifts in incoherent fields, laser fluctuation-induced line splitting, and ac-Stark splitting in stochastic fields with non-Gaussian statistics. A theory is developed which considers the change of classical light statistics during propagation in a nonlinear medium.

*601,456*
**PB86-210739** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Precise Wavelength Measurements and Optical Phase Shifts. 1. General Theory.**
Final rept.,
W. Lichten. 1985, 8p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of the Optical Society of America A2, n11 p1869-1876 Nov 85.

Keywords: *Wavelengths, Phase shift, Optical measurement, Mirrors, Length, Standards, Reprints.

The measurement of wavelengths is subject to systematic errors caused by phase shifts on reflection. The paper gives methods for calculating these phase shifts for metallic and dielectric mirrors from knowledge of the easily obtained reflectivity or transmission spectrum. The Kramers-Kronig relations, as originated by H. W. Bode (Network Analysis and Feedback Amplifier Design (Van Nostrand, Princeton, N.J., 1945)), apply to dielectric and metallic mirrors in many cases. The success of metallic surfaces for interferometry is a direct consequence of the Kramers-Kronig relations. A specific example of a phase-shift calculation for a multilayer-dielectric-coated mirror is given.

*601,457*
**PB86-212909** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Optical Bistability Experiments Using Samarium Vapor.**
Final rept.,
W. J. Sandle, and C. Parigger. 1986, 4p
Pub. in Proceedings of the Topical Meetings on Optical Bistability II, Tucson, AZ., December 2-4, 1985, p231-234 1986.

Keywords: *Samarium, Zeeman effect, Sodium, *Optical bistability, Optical switching.

Experimental investigations of optical bistability (OB) and generalized optical switching for atomic systems with degenerate lower states have up to now relied principally on atomic sodium. Many nonlinear mechanisms have been involved. Except in the simplest cases, the complicated level structure of sodium renders exact theoretical descriptions of these mechanisms beyond effective reach. Furthermore, the number of mechanisms simultaneously involved in the experiments frequently exceeds one. Consequently, one would like to study optical switching in a system for which the number of mechanisms is limited, and for which comparison with exact theoretical description is possible.

*601,458*
**PB86-229804** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Transfer Standards for Energy and Peak Power of Low-Level 1.064 Micrometer Laser Pulses and Continuous Wave Laser Power.**
Final rept.,
A. L. Rasmussen, and A. A. Sanders. 1986, 9p
Pub. in Optical Engineering 25, n2 p277-285 Feb 86.

Keywords: *Standards, Near infrared radiation, Light pulses, Optical measurement, Photodiodes, Continuous radiation, Reprints, *Laser radiation, PIN diodes, Acoustooptics, Optical modulators, Neodymium lasers, YAG lasers.

For the first time, traceable transfer standards have been developed for measuring 1.064 micrometer laser pulses with duration of about 10 to 100 ns, peak power

density of about 10 to the -8th power to 10 to the -4th power W/sq cm, and energy density of about 10 to the -16th power to 10 to the -11th power J/sq cm. These power and energy transfer standards use avalanche (APD) and PIN silicon photodiode detectors, respectively. They are stable and have total uncertainties of about 10%. The system for calibrating them and other devices consists of a cw Nd:YAG laser beam acousto-optically modulated to provide low-level laser pulses of known peak power and energy.

*601,459*
**PB86-229937** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Index of Refraction of Sapphire between 24 and 1060C for Wavelengths of 633 and 799 nm.**
Final rept.,
J. Tapping, and M. L. Reilly. May 86, 7p
Pub. in Jnl. of the Optical Society of America A 3, n5 p610-616 May 86.

Keywords: *Sapphire, Single crystals, Near infrared radiation, Reprints, *Refractive index.

The index of refraction of the ordinary ray in sapphire for temperatures from 24 to 1060 C and for wavelengths of 633 and 799 nm was found to be expressed to 0.02% (99% confidence level). These expressions were calculated from measurements of the relative change with temperature in the reflectance for a plane surface normal to the c axis of single-crystal sapphire.

*601,460*
**PB86-231594** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Determining the Mode-Field Diameter of Single-Mode Optical Fiber: An Interlaboratory Comparison.**
Final rept.,
D. L. Franzen, and R. Srivastava. Oct 85, 5p
Pub. in Jnl. of Lightwave Technology LT-3, n5 p1073-1077 Oct 85.

Keywords: *Fiber optics, Near infrared radiation, Optical measurement, Diameters, Reprints, *Optical fibers, Intercomparison.

The National Bureau of Standards, in cooperation with the Electronic Industries Association, conducted an interlaboratory measurement comparison among fiber manufacturers. Evaluated were transverse splice offset, near-field, far-field, and variable aperture far-field methods for determining mode-field diameter. Measurements were performed on five single-mode fibers at both 1300- and 1550-nm wavelengths. At 1300 nm, agreement was fairly good with the average one standard deviation being 0.15 micrometer for mode-field diameters in the 8-11 micrometer range. Distinct systematic differences among various techniques were observed at 1550 nm where mode distributions are not as Gaussian.

*601,461*
**PB86-231602** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Determining the Effective Cutoff Wavelength of Single-Mode Fibers: An Interlaboratory Comparison.**
Final rept.,
D. L. Franzen. Feb 85, 7p
Pub. in Jnl. of Lightwave Technology LT-3, n1 p128-134 Feb 85.

Keywords: *Fiber optics, Near infrared radiation, Optical measurement, Reprints, *Cutoff wavelength, *Optical fibers, Intercomparison, Cut-off.

The National Bureau of Standards (NBS), in cooperation with the Electronic Industries Association, conducted an interlaboratory measurement comparison among six fiber manufacturers to determine the effective cutoff wavelength of single-mode fibers. Measurement techniques based on transmitted power were used to determine cutoff wavelength on four fibers designed for single-mode operation at 1300 nm. NBS also contributed results using a spectral near-field technique. One standard deviation measurement spreads for the various techniques range from 6 to 12 nm. With the appropriate data analysis, single bend attenuation and power step methods give the same results. Both techniques are easily implemented as extensions to the usual spectral attenuation measurement.

*601,462*
**PB86-231628** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Optical Time-domain Reflectometer Specifications and Performance Testing.**
Final rept.,
B. L. Danielson. 1985, 10p
Pub. in Applied Optics 24, n15 p2313-2322, 1 Aug 85.

Keywords: *Reflectometers, Backscattering, Fiber optics, Performance, Reprints.

From a researcher's as well as a user's point of view, it is highly desirable to adopt a common basis for specifying optical time-domain reflectometer performance parameters. The paper proposes some procedures and test methods which permit these devices to be characterized in a consistent way. Passive test fixtures are also described which may facilitate measurements of dynamic range and other reflectometer properties.

*601,463*
**PB86-241981** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Interlaboratory Measurement Comparison among Fiber Manufacturers to Determine the Effective Cutoff Wavelength and Mode Field Diameter of Single-Mode Fiber.**
Final rept.,
D. L. Franzen. 1985, 1p
Pub. in OFC/OFS '85 - Technical Digest, San Diego, CA., February 11-14, 1985, p36.

Keywords: *Fiber optics, Wavelengths, Diameters, Reprints, *Optical fibers, Intercomparison, Cutoff wavelength.

An interlaboratory measurement comparison to determine an effective cutoff wavelength and mode field diameter of a single-mode fiber was conducted by the National Bureau of Standards in cooperation with the Electronic Industries Association (EIA). Participants include NBS, several U.S. manufacturers, and some foreign laboratories. The purpose of the comparisons is to gather information on interlaboratory agreement when the same measurement techniques are used and to determine systematic offsets between different techniques. The various procedures tested are currently pending before the EIA and represent current practice for manufacturers.

*601,464*
**PB86-242013** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Scratch Standard Is Only a Cosmetic Standard.**
Final rept.,
M. Young. Nov 85, 3p
Pub. in Laser Focus/Electro-Optics, p138-140 Nov 85.

Keywords: *Optical measurement, *Standards, *Surfaces, Reprints, *Scratch and dig standards.

The report presents a history of the scratch and dig standard, describing its application and pointing out that it may not be used for quantitative assessments such as width measurement.

*601,465*
**PB86-245727** PC **A04**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD.
**Holmium Oxide Solution Wavelength Standard from 240 to 640 nm - SRM 2034,**
V. R. Weidner, R. Mavrodineanu, K. D. Mielenz, R. A. Velapoldi, and K. L. Eckerle. Jul 86, 73p NBS/SP-260/102
See also PB86-227592. Also available from Supt. of Docs as SN003-003-02751-1. Library of Congress catalog card no. 86-600560.

Keywords: *Wavelengths, *Standards, Spectrophotometers, Calibrating, Bandwidth, Transmittance, Perchloric acid, Solutions, *Holmium oxides, *Standard reference materials.

The work describes the methods and procedures used to determine the wavelengths of minimum transmittance of holmium oxide in perchloric acid solution. Measurements of spectral transmittance of the solutions were made by means of a high precision spectrophotometer over the wavelength range 200 nm to 680 nm. The wavelength scale accuracy of this instrument was verified by extensive measurements of mercury and deuterium emission lines. The measurements of spectral transmittance of the holmium oxide solutions were made as a function of temperature, purity, concentration, and spectral bandwidth. Analysis of the uncertainties associated with these parameters and the uncertainties associated with the calibration of the instrument wavelength scale and the data analysis have resulted in an estimated uncertainty of + or -0.1 nm for the determination of the wavelengths of minimum transmittance of the holmium oxide solution.

*601,466*
**PB87-103289** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Attenuation Measurements on Deformed Optical Fibers,**
A. Engelsrath, B. L. Danielson, and D. L. Franzen. Jul 86, 33p NBSIR-86/3052

Keywords: *Fiber optics, Optical measurement, Attenuation, Losses, Bending, Tension, Twisting, *Optical fibers, Multimode, Overlap.

Attenuation measurements were made on several different optical fibers subjected to bending, tension, twisting, and overlapping. The measurements were performed with an optical time-domain reflectometer which gives a partial separation between the various contributions to the measured deformation loss. The graded and step-index multimode fibers had a variety of different dimensions and coatings. The results of bending attenuation are compared with models and other reported experimental loss data. Based on the results of the present experiments, an empirical model has been derived which permits a prediction of the smallest bend radius consistent with a given allowed attenuation.

*601,467*
**PB87-104055** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**High-Resolution VUV Spectrometer with Electronic Parallel Spectral Detector.**
Final rept.,
C. Cromer, J. M. Bridges, T. B. Lucatorto, and J. R. Roberts. 1984, 13p
Pub. in American Institute of Physics Conference Proceedings 119, p180-192 1984.

Keywords: *Ultraviolet spectrometers, *Far ultraviolet radiation, Reprints, Laser-produced plasma, Laser applications.

A new high resolution VUV spectrometer is described for applications in the range 40 to 900. The instrument is comprised of a laser-plasma VUV source, which provides continuum background illumination, a 1.5m grazing incidence spectrometer, and a 1024-channel VUV optical multichannel analyzer (VUV-OMA). The VUV-OMA is of new design, featuring a special resolution enhanced channel electron multiplier array in an overall configuration chosen to optimize the spatial resolution of the detector while maintaining single-photoelectron sensitivity. The characteristics of the source and detector along with various applications of the instrument to atomic physics is discussed.

*601,468*
**PB87-104956** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Scratch-and-Dig Standard Revisited.**
Final rept.,
M. Young. 15 Jun 86, 8p
Sponsored by Army Armament Research and Development Command, Dover, NJ., and Department of Defense Calibration Coordination Group, Redstone Arsenal, AL.
Pub. in Applied Optics 25, n12 p1922-1929, 15 Jun 86.

Keywords: *Surfaces, *Standards, *Optical measurement, Diffraction, Reprints, *Scratch and Dig standards.

The scratch standard (MIL-O-13830A) is a cosmetic standard effected by a visual comparison with a set of secondary standards that are in turn evaluated by comparison with a set of master standards. Both manufacture and certification of the secondary standards are somewhat unreliable. The paper shows that they can be classified according to the relative power scattered at a relatively small angle and describes experi-

ments with etched gratings that have the appearance of scratches but diffract light into a broad peak between 5 and 10 degrees off the axis of the incident beam. Some prototypes have been classified both by comparison to the master standards and by a photoelectric measurement; agreement between the two methods is good. Such gratings, used as the secondary standards, should display less intersample variation than scribed or other artifacts. The paper concludes by presenting evidence that the original primary standards have been stable over a long time.

*601,469*
**PB87-105193** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**High-Resolution Spectra of Laser Plasma Light Sources in the Grazing Incidence Region.**
Final rept.,
P. Gohil, V. Kaufman, and T. J. McIlrath. 1986, 2p
Contract F496201-83-C-0130
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Applied Optics 25, n13 p2039-2040, 1 Jul 86.

Keywords: Far ultraviolet radiation, Reprints, *Laser-produced plasma, *Copper plasma, *Ytterbium plasma, *Tungsten plasma, *Light sources.

A Nd:YAG laser has been used to produce plasmas of Cu, Yb, and W. These plasmas were observed with high resolution using the NBS 10.7 m grazing incidence spectrograph. The Yb and W emissions are shown to be excellent sources of continua with very few emission lines.

*601,470*
**PB87-106761** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Investigation of a Laser-Produced Plasma VUV Light Source.**
Final rept.,
J. M. Bridges, C. L. Cromer, and T. J. McIlrath. 1986, 7p
Contract F49620-83-C-0130
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Applied Optics 25, n13 p2208-2214, 1 Jul 86.

Keywords: *Far ultraviolet radiation, Radiometry, Reprints, *Laser-produced plasma, *Light sources, YAG lasers.

An investigation was conducted on the VUV radiation from laser-produced plasmas using a channel electron multiplier detector and a 1.5-m grazing incidence spectrometer. High-resolution quantitative spectra from 8 to 40 nm were obtained from the plasmas generated by a 0.5-J Nd:YAG laser focused on nine different target materials. The effects on the plasma emission of laser energy and focus were measured.

*601,471*
**PB87-107314** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Stabilized Lasers.**
Final rept.,
T. Baer, and J. L. Hall. 1981, 8p
Pub. in Proceedings of Workshop on Precision Doppler Velocity Measurements in Astronomy, Solar Instrumentation - What's Next, Sunspot, NM., October 14-17, 1980, p142-149 1981.

Keywords: *Helium neon lasers, Stabilization.

Two methods of stabilizing He-Ne lasers are described, which provide a wavelength reference with a stability of better than 10 to the -9th power.

*601,472*
**PB87-108684** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Pulse Spectrum Analysis Method of Measuring Fiber Bandwidth.**
Final rept.,
Y. Shao, R. Alvarez, C. Weimer, and R. L. Gallawa. 1985, 4p
Pub. in SPIE Fiber Optics: Short-Haul and Long-Haul Measurements and Applications II 559, p207-210 1985.

Keywords: *Fiber optics, *Bandwidth, Spectrum analysis, Signal to noise ratio, Optical communication, Reprints, *Optical fibers, Multimode.

A system for measuring optical fiber bandwidth using the Pulse Spectrum Analysis method (PSA) has been established. The paper discusses problems inherent to that system such as signal-to-noise ratio and off-peak error. Included are the results of bandwidth measurements on multimode telecommunication grade fibers. Finally, the PSA method is compared to other bandwidth measurement methods: the frequency domain (FD) method, and the time domain (TD) method.

*601,473*
**PB87-108692** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Comparison of Three Bandwidth Measurement Techniques for Multimode Optical Fibers.**
Final rept.,
Y. Shao, and R. L. Gallawa. Jun 86, 8p
Pub. in IEEE Transactions on Instrumentation and Measurement IM-35, n2 p187-194 Jun 86.

Keywords: *Fiber optics, *Bandwidth, Comparison, Reprints, *Optical fibers, Multimode.

The paper presents the results of an experiment intended to compare three distinct methods of measuring the bandwidth of a telecommunication grade, multimode optical fiber. The three methods are: (1) the time-domain method; (2) the frequency-domain method; and (3) the pulse-spectrum analysis method. Good agreement was found between the frequency-domain method and the pulse-spectrum analysis method, but the time-domain method yields results that are lower than the other two for the cases considered.

*601,474*
**PB87-111092** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Precise Wavelength Measurements and Optical Phase Shifts. 2. Applications.**
Final rept.,
W. Lichten. 1986, 7p
Grants NSF-PHY82-17458, NSF-PHY84-19105
See also PB86-210739. Sponsored by National Science Foundation, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in Jnl. of the Optical Society of America A 3, n7 p909-915 Jul 86.

Keywords: *Wavelengths, Phase shift, Optical measurement, Mirrors, Reflection, Length, Standards, Reprints.

The paper calculates the optical phase shifts on reflection from dielectric coated mirrors. The technique consists of measuring the transmission spectrum of the mirrors. These data are fitted with a theoretical expression based on an equivalent, quarter-wave stack. This expression then gives the phase-shift corrections for the mirrors. A fast algorithm, based on a series representation for Chebyshev polynomials, calculates the reflectivity and phase shift for a single wavelength in 3 sec in BASIC on an inexpensive home computer. An application is to measure absolute wavelengths with equipment commonly present in laser laboratories, namely, scanning Fabry-Perot interferometers with dielectric coated mirrors. The method is that of exact fractions, which requires one primary wavelength standard, with a less accurate, secondary standard (or wavemeter). The accuracy of the technique is equal to that of the primary standard. The precision is that of reading the interferometer and can be many times that of the secondary standard.

*601,475*
**PB87-117727** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Calibration in 1976 and 1983 of Didymium Glass Filters Issued as NBS (National Bureau of Standards) Standard Reference Materials.**
Final rept.,
K. L. Eckerle, S. Chang, and J. J. Hsia. 1985, 6p
Pub. in Color Research and Application 10, n1 p32-37 1985.

Keywords: *Optical filters, *Standards, *Spectrophotometers, *Calibrating, Wavelengths, Reprints, *Standard reference materials, Uncertainty.

In 1983, a new supply of didymium glass filters was prepared, as the stock calibrated in 1976 have been very useful and the inventory has been depleted. Results for representative samples of the new filters are presented. The new supply of glass has been calibrated by the batch mode and will be designated Standard Reference Materials (SRM) 2009A and 2010A. During the latter part of 1976, research was begun to characterize didymium glass filters for use with spectrophotometers with bandwidth in the range 1.5 to 10.5 nm. These filters were to have a smaller uncertainty than previously issued filters. Also, it was found that points of inflection in the transmittance curve could be used to supplement the data for transmittance minima. The results of that research were SRM 2009, 2010, 2013, and 2014. The same techniques were applied in 1983. Also, the results from 1983 and 1976 for one of the Master filters are compared.

*601,476*
**PB87-118329** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Scanning Tunneling Microscopy Applied to Optical Surfaces.**
Final rept.,
R. A. Dragoset, R. D. Young, H. P. Layer, S. R. Mielczarek, and E. C. Teague. 1986, 3p
Pub. in Optics Letter 11, n9 p560-562 Sep 86.

Keywords: *Optical measurement, *Surface roughness, Gratings(Spectra), Mirrors, Reprints, *Scanning tunneling microscopy, Diamond turning.

The technique of scanning tunneling microscopy has been applied to topographic mapping of two optical surfaces: a ruled grating replica and a diamond-turned gold mirror. The authors have demonstrated the ability of the scanning tunneling microscope to measure surface topography of a ruled-grating replica over an area of 2 micrometers X 2 micrometers. Furthermore, surface structure on a diamond-turned gold mirror was observed that could not be detected by any other type of surface-sensitive microscope. These measurements yield information necessary for gaining a complete understanding of the diamond-turning process.

*601,477*
**PB87-121323**
(Order as PB87-121315, PC **A04**/MF **A01**)
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Wavelength Standard for the Near Infrared Based on the Reflectance of Rare-Earth Oxides,**
V. R. Weidner, P. Y. Barnes, and K. L. Eckerle. 29 Feb 85, 11p
Included in Jnl. of Research of the National Bureau of Standards, v91 n5 p243-253 Sep-Oct 86.

Keywords: *Near infrared radiation, *Standards, Reflectance, Erbium oxides, Bandwidth, *Wavelength standards, Dysprosium oxides, Holmium oxides.

The work describes the techniques used to prepare and analyze a reflectance wavelength standard composed of three rare-earth oxides. A mixture of dysprosium oxide ($Dy_2O_3$), erbium oxide ($Er_2O_3$), and holmium oxide ($Ho_2O_3$) provides a pressed powder specimen exhibiting a near infrared reflectance spectrum charactrerized by many discrete absorption minima in the wavelength range 700 to 2000 nm. The object of this activity was to develop a wavelength standard for improving the accuracy of reflectance measurements in the near infrared.

*601,478*
**PB87-122453** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Pub. in Fiber Bandwidth Measurement Using Pulse Spectrum Analysis.**
Final rept.,
Y. Shao, and R. L. Gallawa. 1986, 3p
Applied Optics 25, n7 p1069-1071, 1 Apr 86.

Keywords: *Fiber optics, *Bandwidth, Spectrum analysis, Comparison, Reprints, *Optical fibers, Time domain, Frequency domain.

The pulse spectrum analysis (PSA) method of measuring fiber bandwidth has been suggested as an alternative to the frequency and time domain methods, but there is a paucity of information on the technique and very little data. In fact, we know of no measurement comparisons between the PSA method and the frequency and time domain methods. The PSA method has the advantage of being very simple and gives results that are consistent with the time domain and frequency domain methods. The International Electro-

technical Commission (IEC) recommends the PSA method, but the Electronics Industries Association (EIA) of the U.S.A. takes no position in this regard. The paper gives results of an experiment which compared the three methods.

*601,479*
**PB87-122628** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Single-Mode Fiber Dispersion Measurements Using Optical Sampling with a Mode-Locked Laser Diode.**
Final rept.,
T. Kanada, and D. L. Franzen. 1986, 3p
Pub. in Optics Letters 11, n5 p330-332 May 86.

Keywords: *Laser beams, *Optical dispersion, Light pulses, Fiber optics, Reprints, Mode locked lasers, Optical fibers.

Pulses from a wavelength-tunable, mode-locked laser diode were measured after 21 km of single-mode fiber propagation by optical sampling with another mode-locked laser diode; a resolution of 0.1 psec/(nm km) is achieved in the chromatic dispersion measurement. In another related experiment, 78-psec-duration pulses from an oedinary, multilongitudinal-mode laser diode are clearly displayed by optical sampling after 36 km of fiber propagation. System bandwidth increases to approximately 500 GHz km as the laser-diode wavelength is temperature tuned through the zero-dispersion region.

*601,480*
**PB87-122636** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Optical Waveform Measurement by Optical Sampling with a Mode-Locked Laser Diode.**
Final rept.,
T. Kanada, and D. L. Franzen. 1986, 3p
Pub. in Optics Letters 11, n1 p4-6 Jan 86.

Keywords: *Laser beams, *Waveforms, *Optical measurement, Reprints, Aluminum gallium arsenide lasers, Gallium indium arsenide phosphide lasers, Optical fibers, Lithium iodates, Mode locked lasers.

Optical pulses from a GaAlAs laser diode directly modulated at a frequency fo (971 MHz) are mixed in a LiIO3 crystal with optical sampling pulses at a frequency of fo - 10 Hz from a mode-locked GaAlAs laser diode. The optical signal obtained by sum-frequency mixing in the crystal is observed with a photomultiplier and an oscilloscope. The original pulse waveform is reproduced clearly with a temporal resolution equal to the mode-locked laser-diode pulse width and at a repetition frequency of 10 Hz. Similar results are obtained with InGaAsP laser diodes at a wavelength of 1.3 micrometers.

*601,481*
**PB87-122644** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Direct Measurement of the Spatial Modes of a Laser Pulse: Theory.**
Final rept.,
E. G. Johnson. 1986, 9p
Sponsored by Department of Defense Calibration Coordination Group, Redstone Arsenal, AL.
Pub. in Applied Optics 25, n17 p2967-2975, 1 Sep 86.

Keywords: *Laser beams, *Electric fields, Light pulses, Fiber optics, Reprints, Beam profiles, Optical fibers.

An electric-field measuring apparatus was made by using optical processing, tapered optical fibers, and a pair of detectors at the end of each optical fiber. Using an appropriate computer-generated hologram (CGH), the author shows it is possible to discriminate among a set of orthonormal modes used to represent the spatial features of the electric field with a SNR of at least 100 to 1. The tapered fiber is a mode filter that is used in the transform plane of the CGH. The fiber allows precise determination of the strength of each of the orthonormal modes being used as the spatial basis of the electric field before the optical processing.

*601,482*
**PB87-122677** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Linearity Study of a Diode-Array Radiometer.**
Final rept.,
A. T. Hattenburg, and J. B. Shumaker. 1984, 2p
Pub. in Applied Optics 23, n19 p3257-3258 1984.

Keywords: *Radiometers, Arrays, Photodiodes, Linearity, Silicon, Detectors, Spectroradiometers, Reprints.

No abstract available.

*601,483*
**PB87-122685** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Comparison of the NBS SURF (National Bureau of Standards Synchrotron Ultraviolet Radiation Facility) and Tungsten Ultraviolet Irradiance Standards.**
Final rept.,
H. J. Kostkowski, J. L. Lean, R. D. Saunders, and L. R. Hughey. 1986, 10p
Pub. in Applied Optics 25, n18 p3297-3306, 15 Sep 86.

Keywords: *Irradiance, *Standards, Near ultraviolet radiation, Comparison, Reprints, Synchrotron Ultraviolet Radiation Facility.

Detailed comparisons of the spectral irradiance of the NBS Synchrotron Ultraviolet Radiation Facility II and tungsten FEL Scale of Spectral Irradiance at 297 and 254 nm with an uncertainty of about 1% show that these irradiance standards are consistent at both wavelengths to within the uncertainties assigned to them by NBS.

*601,484*
**PB87-125738** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Metrology for Electromagnetic Technology: A Bibliography of NBS (National Bureau of Standards) Publications,**
K. E. Kline, and M. E. DeWeese. Jun 86, 57p NBSIR-86/3048
Supersedes PB86-130234.

Keywords: *Electromagnets, *Metrology, *Fiber optics, *Bibliographies, Lasers, Optical communication, Superconductors, Standards, *Cryoelectronics, National Bureau of Standards.

The Electromagnetic Technology Division was formed during the reorganization of NBS in April 1978 by combining parts of the former Electromagnetics and Cryogenics Divisions. It develops measurement methods and standards and provides metrological support for: laser systems; optical communication equipment; cryoelectronics; superconductors; and other unusual electrical engineering materials.

*601,485*
**PB87-128054** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Optical Frequency Measurements.**
Final rept.,
D. A. Jennings, K. M. Evenson, and D. J. E. Knight. 1986, 12p
Pub. in Proceedings of the Institute of Electrical and Electronics Engineers 74, n1 p168-179 Jan 86.

Keywords: *Frequency measurement, Dimensional measurement, Length, Standards, Reprints, *Laser radiation, Light speed.

The paper is a review of the history of the measurement of coherent optical frequencies. As coherent optical frequency implies a laser device, this is therefore a review of laser frequency measurement. The development of frequency measurement from the Cs frequency standard to the visible is traced. Two related aspects of optical frequency measurements, the speed of light and the redefinition of the meter, are also discussed.

*601,486*
**PB87-128112** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Angular Momentum of Trapped Atomic Particles.**
Final rept.,
D. J. Wineland, J. J. Bollinger, W. M. Itano, and J. D. Prestage. 1985, 10p
Sponsored by Office of Naval Research, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of the Optical Society of America B 2, n11 p1721-1730 Nov 85.

Keywords: Angular momentum, Radiation pressure, Reprints, *Ion traps, *Atom traps, Ion storage, Laser spectroscopy, Laser cooling.

In axially symmetric atomic-particle traps, the angular momentum of the particles about the symmetry axis is conserved in the absence of external torques. Changes in this angular momentum owing to laser scattering are discussed.

*601,487*
**PB87-128997** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Intercomparison between Independent Irradiance Scales Based on Silicon Photodiode Physics, Gold-Point Blackbody Radiation, and Synchrotron Radiation.**
Final rept.,
A. R. Schaefer, R. D. Saunders, and L. R. Hughey. 1986, 5p
Pub. in Optical Engineering 25, n7 p892-896 Jul 86.

Keywords: *Irradiance, *Radiometry, Synchrotron radiation, Photodiodes, Reprints, Intercomparison.

An intercomparison has been conducted among three independent scales of spectral irradiance: two source-based and one detector-based. Specifically, a radiometer composed of a silicon photodiode, an interference filter, and an integrating sphere was characterized and calibrated against an absolute silicon detector standard at 600 nm using a cw dye laser. The radiometer was then used to measure the spectral irradiance at 600 nm from spectral irradiance lamps calibrated against a gold-point blackbody, and the spectral irradiance at the same wavelength from the NBS electron storage ring, SURF-II. Intercomparisons of this type are an important check of the agreement between these independent radiometric techniques. It was found that the detector scale indicated a spectral irradiance at 600 nm that was 0.76% lower than predicted by the gold-point blackbody scale and 0.25% higher than predicted by the electron storage ring scale. This result implies agreement within the overall quadrature uncertainties of plus of minus 0.25% for the detector scale, plus or minus 0.84% for the gold-point blackbody scale, and plus or minus 0.60% for the electron storage ring scale.

*601,488*
**PB87-133294** PC **A08**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Technical Digest - Symposium on Optical Fiber Measurements, 1986,**
G. W. Day, and D. L. Franzen. Sep 86, 159p NBS/SP-720
See also PB85-114700. Also available from Supt. of Docs as SN003-003-02772-3. Library of Congress catalog card no. 86-600563. Prepared in cooperation with Institute of Electrical and Electronics Engineers, Inc., New York, and Optical Society of America, Washington, DC.

Keywords: *Fiber optics, *Meetings, Optical measurement, Dimensional measurement, Diameters, Electrooptics, Optical communication, *Optical fibers, Multimode.

The digest contains summaries of 34 papers presented at the Symposium on Optical Fiber Measurements, held September 9-10, 1986, at the National Bureau of Standards, Boulder, Colorado.

*601,489*
**PB87-134193** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Excited-State Stability and X-ray Lasers.**
Final rept.,
J. N. Bardsley. 1986, 2p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Optics Letters 11, n10 p612-613 Oct 86.

Keywords: Stability, Reprints, *X ray lasers, Multiphoton processes.

Based on the results of recent studies of microwave ionization of Rydberg states, estimates are obtained for the stability of excited states of highly charged ions under irradiation from a powerful excimer laser. The short lifetimes and associated line broadening suggest

caution in the design of x-ray lasers using selective multiphoton excitation as a pumping mechanism.

*601,490*
**PB87-134920** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Pressure Effects on the Frequency of Continuous-Wave Optically Pumped Far-Infrared Lasers.**
Final rept.,
M. Inguscio, and K. M. Evenson. 1984, 2p
Pub. in Optics Letters 9, n10 p443-444 1984.

Keywords: *Infrared lasers, Far infrared lasers, Frequencies, Reprints, Pressure dependence.

The frequency of the 170.6 micrometer cw CH(3)OH optically pumped laser emission has been remeasured at different pressures without observing the pressure shift observed by Lawandy and Koepf. The FIR frequency was synthesized with two stabilized CO2 lasers. No measurable pressure shift over the operating pressure range of the laser was observed, and the frequency was confirmed to be 1757526.3 MHz. However, competing lasing lines were found to produce spurious effects on the frequency. These may explain their apparent shifts.

*601,491*
**PB87-136644** PC **A19**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Laser Induced Damage in Optical Materials: 1984.**
Special pub. (Final),
H. E. Bennett, A. H. Guenther, D. Milam, and B. E. Newnam. Oct 86, 448p NBS/SP-727
See also PB82-112921. Also available from Supt. of Docs as SN003-003-02761-8. Library of Congress catalog card no. 86-600587. Sponsored by American Society for Testing and Materials, Philadelphia, PA., Office of Naval Research, Arlington, VA., Department of Energy, Washington, DC., and Defense Advanced Research Projects Agency, Arlington, VA.

Keywords: *Optical materials, *Laser materials, *Meetings, *Radiation damage, Mirrors, Surfaces, Thin films, Infrared radiation, Ultraviolet radiation, Optical coatings, *Physical radiation effects, Laser damage, Picosecond pulses.

The Symposium was divided into sessions concerning Materials and Measurements, Mirrors and Surfaces, Thin Films, and Fundamental Mechanisms. As in previous years, the emphasis of the papers presented at the Symposium was directed toward new frontiers and new developments. Particular emphasis was given to materials for high power apparatus. The wavelength range of prime interest was from 10.6 micrometers to the uv region. Highlights included surface characterization, thin film-substrate boundaries, and advances in fundamental laser-matter threshold interactions and damage mechanisms.

## Plasma Physics

*601,492*
**DE85007605** PC **A04**/MF **A01**
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Survey of Experimental and Theoretical Electron-Impact Ionization Cross Sections for Transition Metal Ions in Low Stages of Ionization.**
M. S. Pindzola, D. C. Griffin, C. Bottcher, D. C. Gregory, and A. M. Howald. Mar 85, 64p ORNL/TM-9436
Contract AC05-84OR21400

Keywords: *Copper Ions, *Iron Ions, *Nickel Ions, *Titanium Ions, Cross Sections, *Electron-Ion Collisions, Experimental Data, *Ionization, Theoretical Data, ERDA/700103.

Electron-ion crossed beams measurements and distorted-wave theory have been employed to make a study of electron-impact ionization for transition metal ions in low stages of ionization. The atomic ions Ti+, Ti exp 2 +, Ti exp 3 +, Fe+, Fe exp 2 +, Fe exp 3 +, Fe exp 4 +, Ni+, Ni exp 2 +, Ni exp 3 +, Cu+, Cu exp 2 +, and Cu exp 3 + are examined. (ERA citation 10:017597)

*601,493*
**PB86-192424** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Fokker-Planck and Langevin Descriptions of Fluctuations in Uniform Shear Flow.**
Final rept.,
R. F. Rodriguez, E. Salinas-Rodriguez, and J. W. Dufty. 1983, 20p
Pub. in J. Stat. Phys. 32, n2 p279-298 Aug 83.

Keywords: *Diffusion, Kinetic theory, Langevin equation, Shear flow, Reprints, Fokker-Planck equation.

The Boltzmann description of the preceeding paper for tagged particle fluctuations in a nonequilibrium gas is further analysed in the limit of small mass ratio between the gas and tagged particles. For a large class of nonequilibrium states the Boltzmann-Lorentz collision operator for the tagged particle distribution is expanded to leading order in the mass ratio, resulting in a Fokker-Planck operator. The drift vector and diffusion tensor are calculated exactly for Maxwell molecules. The Fokker-Planck operator depends on the nonequilibrium state only through the hydrodynamic variables for the fluid. The diffusion tensor is a measure of the 'noise' amplitude and is not simply determined from the nonequilibrium temperature; instead, it depends on the fluid stress tensor components as well. For the special case of uniform shear flow, the Fokker-Planck equation is of the linear type and may be solved exactly. The associated set of Langevin equations is also identified and used to describe spatial diffusion in the Langrangian corrdinates of the fluid. The effect of viscous heating on diffusion is discussed and the dependence of the diffusion coefficient on the shear rate is calculated.

*601,494*
**PB86-193844** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Plasma Shifts of the He II (H sub alpha) and (P sub alpha) Lines.**
Final rept.,
T. L. Pittman, and C. Fleurier. 1986, 6p
Pub. in Physical Review A: General Physics 33, n2 p1291-1296 Feb 86.

Keywords: Emission spectra, Stark effect, Reprints, *Helium plasma, Line broadening.

Shift measurements for the H(alpha)(1640 A) and (P alpha) (4686 A) hydrogenic ion lines of He II have been done over an electron density range 2 x 10 to the 22nd power to 2 x 10 to the 23rd power/cu m and for an electron temperature of 4 eV. The plasma was produced in a linear Z discharge. Systematic red shifts linear in density are observed. The experimental data are compared with combined theoretical estimates for electron-impact and ion quadrupole effects. The experimental results are in agreement with their earlier results for Pa.

*601,495*
**PB86-195591** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Study of Hydrogen Stark Profiles by Means of Computer Simulation.**
Final rept.,
R. Stamm, E. W. Smith, and B. Talin. Oct 84, 8p
Pub. in Physical Review A 30, n4 p2039-2046 Oct 84.

Keywords: Computerized simulation, Line spectra, Reprints, *Hydrogen plasma, Lyman lines.

A computerized simulation technique is used to calculate hydrogen spectral lines emitted by a plasma. These calculations are used to study ion dynamic effects on the line profiles. Results are obtained for Lyman alpha, Lyman beta and Lyman gamma lines, and comparisons are made with experimental results and with other theoretical methods.

*601,496*
**PB87-130530** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Shifts of Ion Lines in Plasmas.**
Final rept.,
D. E. Kelleher, and J. Cooper. 1985, 36p
Pub. in Spectral Line Shapes, p85-120 1985.

Keywords: *Plasma(Physics), Polarization, Reprints, Shift.

A review of the experimental and theoretical aspects of the topic is presented. The authors begin with a brief summary of the subject's history. An overview of the current experimental situation for hydrogenic and 'isolated' ion lines will preceed an informal discussion of a recent formal theoretical approach to the problem. An important conclusion of the theory is that the 'plasma polarization' shift does not exist in the following sense: If one properly includes the effects of ion fields and of electron collisions in their nearly hyperbolic paths, then all the relevant physics is accounted for. The main difficulty in making accurate calculations of the shift is to properly account for strong collisions. A close coupling calculation should address many of the unanswered questions, such as the importance of low l partial waves and exchange. Current efforts being made in the direction are described.

## Radiofrequency Waves

*601,497*
**PB86-197191** PC **A06**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**SCAT: A Vector Program to Solve a Transient MFIE (Magnetic Field Integral Equation),**
E. Marx. Apr 86, 105p NBSIR-86/3362

Keywords: *Computer programs, *Electromagnetic scattering, Magnetic fields, Integral equations, Mie scattering, SCAT computer program.

The FORTRAN program SCAT is used to solve the magnetic field integral equation (MFIE) to determine the fields scattered by a perfectly conducting sphere. The incident field is a plane-wave pulse, and a stepping-in-time procedure is used to determine the surface current density induced on the sphere. The program does not take advantage of the special symmetry of the scatterer because it is intended to serve as a verified starting point for more general programs. The output is compared to that of the program PERF, which computes the same fields via a Fourier transform of the monochromatic fields obtained from the Mie formulas. The contributions of the self-patch and neighboring patches to the singular integral are optionally computed by using their expansions in the linear size of the patches. The self-patch term is important for the solution of other integral equations that may be of the first kind. For the MFIE, these corrections are small but not negligible. The program takes advantage of the vector programming features of the CYBER 205.

*601,498*
**PB87-134359** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Lattice Approach to Volumes Irradiated by Unknown Sources,**
J. Randa, and M. Kanda. Oct 86, 64p NBS/TN-1303
Also available from Supt. of Docs as SN003-003-02778-2.

Keywords: *Electromagnetic environments, Electromagnetic fields, Action principle, Ill posed problems, Successive overrelaxation method, Numerical solution.

The authors suggest an approach to the characterization of electromagnetic environments irradiated by unknown sources. The approach is based on the numerical solution of Maxwell's equations subject to the constraints imposed by the measured values of the field at a small number of measurement points and by boundary conditions. A thorough examination of two methods for the numerical solution is presented. The examples attempted demonstrate the approach but reveal that neither technique is fully successful. Possible future directions are suggested.

## Solid State Physics

*601,499*
**PB86-160728** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

**Electron Tunneling into Superconducting Filaments Using Mechanically Adjustable Barriers.**
Final rept.,
J. Moreland, and J. W. Ekin. Jul 85, 3p
Contract DE-AI01-84ER52113
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Applied Physics Letters 47, n2 p175-177, 15 Jul 85.

Keywords: *Superconductors, *Electron tunneling, Niobium, Energy gap, Filaments, Reprints.

A new type of squeezable tunneling (SET) junction has been developed for tunneling into superconducting filaments. Stable, mechanically adjustable tunneling barriers between the native surfaces of sputtered Nb films and 30-micrometers-diam Nb filaments were established in liquid helium at 4 K. The current versus voltage characteristics of these SET junctions were used to determine the superconducting energy gap at the surface of the filaments. Since the filaments were etched from commercial superconducting magnet wire, the type of tunnel junction shows promise as a diagnostic probe of superconducting materials for high-field magnets.

*601,500*
**PB86-162120** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Electron Tunneling Experiments Using Nb-Sn 'Break' Junctions.**
Final rept.,
J. Moreland, and J. W. Ekin. 15 Nov 85, 8p
Contract DE-AI01-84ER52113
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy, and National Research Council, Washington, DC.
Pub. in Jnl. of Applied Physics 58, n10 p3888-3895, 15 Nov 85.

Keywords: *Superconductors, *Electron tunneling, Energy gap, Reprints, Niobium tin.

An Nb-Sn filament mounted on a flexible glass beam can be broken to form an electron tunneling junction between the fracture elements. Breaking the filament in liquid helium prevents oxidation of the freshly exposed fracture surfaces. A sharp superconducting energy gap in the I-V characteristics measured at 4 K indicates the formation of a high-quality tunneling barrier between the fracture elements. The resistance of the junction can be continuously adjusted by varying the surface bending strain of the beam. An estimated 0.1 nm change in the barrier thickness produces about an order of magnitude change in the resistance over the range from 100,000 to 100 million ohms. The exponential character of the dependence shows that the tunnel junction is freely adjustable without intimate contact of the junction elements. 'Break' junctions made in this way offer a new class of tunneling experiments on freshly exposed surfaces of a fractured sample without the oxide barrier previously required for junction stability. Such experiments provide a simple technique for tunneling to new materials and may eliminate complications that can be encountered during interpretation of data obtained using oxide barriers.

*601,501*
**PB86-163532** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Precision and Accuracy in Structure Refinement by the Rietveld Method.**
Final rept.,
E. Prince. 1985, 9p
Pub. in Structure and Statistics in Crystallography, p95-103 1985.

Keywords: *Crystal structure, Standard deviation, Least squares method, Precision, Accuracy, Bias, Reprints, *Rietveld method, Parameter estimation.

Whenever the values of a set of experimental observations can be predicted by a model containing adjustable parameters, the values of those parameters can be estimated by the method of least squares. Statistical methods may be used to test whether the fitted model is consistent with the data and, on the assumption that the model is the correct one, to estimate the standard deviations of the parameters. Standard deviations, however, are measures of precision rather than of accuracy. Various workers have attempted to assess the accuracy of the method, by defining a number greater than one by which the standard deviations may be multiplied, or by using alternative procedures, such as the separate estimation of integrated intensities or the use of non-diagonal weight matrices. All of these attempts are hampered by the absence in the data, of any information concerning the correlations between systematic errors, and other sources of bias, and the parameters being estimated.

*601,502*
**PB86-164530** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**High Resolution Magnetic Microstructure Imaging Using Secondary Electron Spin Polarization Analysis in a Scanning Electron Microscope.**
Final rept.,
J. Unguris, G. G. Hembree, R. J. Celotta, and D. T. Pierce. Aug 85, 2p
Pub. in Jnl. of Microscopy 139, pt2 pRP1-RP2 Aug 85.

Keywords: Ferromagnetism, Microstructure, Reprints, *Electron spin polarization, Scanning electron microscopy, Imaging techniques, Magnetism.

In recent measurements it was shown that the low energy secondary electrons generated when an electron beam is incident on a ferromagnetic material are spin polarized, reflecting the net spin density of the valance electrons of the ferromagnet (Unguris, et al., 1982). Additionally, it was predicted that the electron spin polarization should provide an efficient contrast mechanism that can be measured simultaneously with but independently of topographical contrast (Unguris, et al., 1982). The prediction was first tested by Koike and Hayakawa (1984, 1985) who used a scanning 10 micrometer diameter electron beam in conjunction with a 100 keV Mott spin analyzer to show that indeed the polarization contrast was large and could be obtained independently of the topographical contrast.

*601,503*
**PB86-185337** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Raman Spectrum of Carbon in Silicon.**
Final rept.,
R. A. Forman, M. I. Bell, D. R. Myers, and D. Chandler-Horowitz. Oct 85, 3p
Contract DE-AC04-76DP00789
Sponsored by Department of Energy, Washington, DC.
Pub. in Japanese Jnl. of Applied Physics 24, n10 pL848-L850 Oct 85.

Keywords: *Silicon, *Carbon, *Raman spectra, Impurities, Infrared spectra, Reprints, Semiconductors.

Raman spectroscopy is used to characterize carbon-doped silicon samples prepared by ion implantation and pulsed laser annealing. Sharp lines are observed in the Raman spectra due to the (12) C local mode at 604 + or - 1/cm and the (13) C local mode at 586 + or -1/cm. Identical spectra are obtained from a given carbon implant whether it is annealed using a 10 ns pulsed ruby laser or the significantly longer pulse of an R6G dye laser. It is shown that Raman spectroscopy has sufficient sensitivity to detect striated carbon distributions in as-grown commercial silicon. Finally, at high carbon density, where the local modes begin to broaden in the implanted and laser-annealed samples, a disorder-induced first-order Raman spectrum is observed produced by the mass defect of the substitutional carbon.

*601,504*
**PB86-185451** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Magnetoplasmon Excitations from Partially Filled Landau Levels in Two Dimensions.**
Final rept.,
A. H. MacDonald, H. C. A. Oji, and S. M. Girvin. Nov 85, 4p
Pub. in Physical Review Letters 55, n20 p2208-2211, 11 Nov 85.

Keywords: Electron gas, Magnetic fields, Excitation, Reprints, *Magnetoplasmons, Heterostructures, Quantum Hall effect.

For a noninteracting two-dimensional electron gas in a strong perpendicular magnetic field, the excitation energies are multiples of (h bar)(omega sub c). These excitation energies are shifted in an interacting system. Because of the singular nature of the noninteracting-system energy spectrum it has previously been possible to evaluate the excitation energies of the interacting system only when all Landau levels are either completely empty or completely full. In the article they suggest a nonperturbative approach which overcomes this difficulty but recovers existing results in the appropriate limits.

*601,505*
**PB86-185865** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Monte Carlo Calculation of One- and Two-Dimensional Particle and Damage Distributions for Ion-Implanted Dopants in Silicon.**
Final rept.,
J. Albers. Oct 85, 10p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in IEEE (Institute of Electrical and Electronic Engineers) Transactions on Electron Devices ED-32, n10 p1930-1939 Oct 85.

Keywords: *Silicon, *Crystal defects, *Radiation damage, Semiconductor doping, Vacancies(Crystal defects), Interstitials, Monte Carlo method, Reprints, *Ion implantion, Physical radiation effects.

The two-dimensional distributions of particles, primary damage, and electronic and nuclear energy loss were calculated for implantation of a line source into silicon targets by using the TRIM Monte Carlo code. In addition, the Kinchin-Pease equation was used to calculate approximate two-dimensional distributions of the Frenkel pairs (vacancy-interstitial) created by the primary displacement damage of the target atoms. These distributions allowed for the calculation of the one-dimensional distributions of these quantities for implantation into unmasked targets. The two-dimensional particle and approximate Frenkel pairs distributions for implantation past a mask edge were constructed by means of superposition. The results are important for understanding the mass, energy, and dose dependence of implantation and the associated displacement damage.

*601,506*
**PB86-186061** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Near Ultraviolet Quantum Yield of Silicon.**
Final rept.,
F. J. Wilkinson, A. J. D. Farmer, and J. Geist. Feb 83, 3p
Pub. in Jnl. of Applied Physics 54, n2 p1172-1174 Feb 83.

Keywords: *Silicon, *Quantum efficiency, *Photodiodes, Near ultraviolet radiation, Reprints, Band theory.

New values for the quantum yield of silicon in the 3 to 5 eV spectral region are derived from reflectance and photo-response measurements on oxide/p+/n/n+ photodiode structures. The new values fall between high and low estimates derived from a recent model of impact ionization phenomena due to Alig, Bloom and Struck. A prominent peak in the new spectrum near 4.5 eV is attributed to the way the photon energy in excess of the band gap energy is distributed between the photo-generated electrons and holes at different photon energies due to the band structure.

*601,507*
**PB86-187739** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Fractional Quantum Hall Effect: Superfluidity, Magneto-Rotons and Fractionally Charged Vortices.**
Final rept.,
S. M. Girvin, A. H. MacDonald, and P. M. Platzman. 1986, 5p
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p1428-1432 1986.

Keywords: *Hall effect, Electron gas, Superfluidity, Reprints, *Fractional Quantum Hall effect, *Quantum Hall effect.

The fractional quantum Hall effect is a remarkable macroscopic quantum phenomenon in which the Hall resitivity of a two-dimensional electron gas is accurately quantized in units of h/(e squared). This nearly dissipationless state is analogous to superfluidity with the collective excitations being phonons, magneto-rotons, and fractionally charged vortices.

*601,508*
**PB86-187747** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Magneto-Roton Theory of Collective Excitations in the Fractional Quantum Hall Effect.**
Final rept.,
S. M. Girvin, A. H. MacDonald, and P. M. Platzman. 15 Feb 86, 14p
Pub. in Physical Review B 33, n4 p2481-2494, 15 Feb 86.

Keywords: *Hall effect, Superfluidity, Reprints, *Fractional Quantum Hall effect, *Quantum Hall effect, Rotons.

The authors present a theory of the collective excitation spectrum in the fractional quantum Hall effect which is closely analogous to Feynman's theory of superfluid helium. The predicted spectrum has a large gap at k=0 and a deep magneto-roton minimum at finite wave vector, in excellent quantitative agreement with recent numerical calculations. They demonstrate that the magneto-roton minimum is a precursor to the gap collapse associated with the Wigner crystal instability occurring near nu=1/7. In addition to providing a simple physical picture of the collective excitation modes, the theory allows one to compute rather easily and accurately experimentally relevant quantities such as the susceptibility and the ac conductivity.

*601,509*
**PB86-187754** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Magnetic Field Dependence of the Small Angle Neutron Scattering in HoMo6Se8.**
Final rept.,
J. A. Gotaas, and J. W. Lynn. 1986, 2p
Grant NSF-DMR83-19936
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p1529-1530 1986.

Keywords: *Superconductors, Neutron scattering, Magnetic fields, Phase transformations, Reprints, *Holium molybdenum selenides, *Magnetic superconductors.

The field dependence of the modulated magnetic state in the superconductor HoMo6Se8 has been investigated using small angle neutron scattering. In zero field there is a single peak at the modulation wave vector (q sub c). A magnetic field induces a separate component at smaller q, with both components becoming increasingly anisotropic with field.

*601,510*
**PB86-188463** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Structure of Dicalcium Potassium Heptahydrogen Tetrakis Phosphate Dihydrate, CA2KH7(PO4)4, 2H20, by X-ray and Neutron-Diffraction.**
Final rept.,
E. Prince, S. Takagi, M. Mathew, and W. E. Brown. 1984, 4p
Pub. in Acta Crystallographica Section C-Crystal Structure Communications 40, p1499-1502 1984.

Keywords: *Crystal structure, Calcium phosphates, X ray diffraction, Neutron diffraction, Chemical bonds, Hydrates, Reprints, *Calcium potassium hydrogen phosphates.

Ca2KH7(PO4)4 . 2H2O, M = 542. 25, triclinic, a = 5.676(1), b = 12.210(2), c = 6.292(1), alpha = 104.10(3) deg, beta = 115.16(2) deg, gamma = 84.25(2) deg, V = 382.79(A cubed), Z = 1, D =2.352 MgM-3. For X-rays, space group P1, lambda = 0.7107, R = 0.024 for 2040 independent observed reflections. For neutrons, space group P1, lambda = 1.273 A. R = 0.051 for 1383 independent observed reflections. The structure is isomorphous with Ca2(NH4)H7(PO4) 4 2H2O. Although K could occupy a center of symmetry, it apparently does not, and two of the three hydrogen bonds that would cross centers of symmetry in P(1 bar) are also markedly asymmetric.

*601,511*
**PB86-189057** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Recent Advances in the Electron Microscopy of Materials.**
Final rept.,
D. B. Williams, and D. E. Newbury. 1984, 128p
Pub. in Advances in Electronics and Electron Physics 62, p161-288 1984.

Keywords: *Electron microscopy, Crystal structure, Crystal defects, Reprints, Transmission electron microscopy, Scanning electron microscopy.

Modern electron microscopy of materials involves a wide range of techniques, including transmission electron microscopy, scanning electron microscopy, scanning transmission electron microscopy, diffraction, and chemical microanalysis. Advances in instrumentation have made a variety of new techniques possible, including analytical electron microscopy, energy dispersive x-ray spectrometry, electron energy loss spectrometry. High resolution imaging of lattice fringes and structures of thin specimens is possible in the TEM and of thick specimens in the SEM. Contrast mechanisms are available for direct imaging of crystallographic, magnetic, electrical and thermal properties of a specimen. Combinations of imaging, diffraction, and analysis techniques provide complete materials characterization.

*601,512*
**PB86-189180** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Impurity Bands and Band Tailing in Moderately Doped Silicon.**
Final rept.,
J. R. Lowney. 1986, 6p
Pub. in Jnl. of Applied Physics 59, n6 p2048-2053, 15 Mar 86.

Keywords: *Silicon, Conduction bands, Valence bands, Energy gap, Impurities, Reprints, *Band theory, Semiconductors, Density of states.

The density of states of the valence and conduction bands in silicon has been calculated at room temperature for dopant densities near the transition between the existence of a distinct impurity band and its coalescence with the continuum band to form a band tail. The dopant densities for the three cases considered are (1) 1.5 X 10 to the 18th power acceptors; (2) 6.2 X 10 to the 18th cm-3 acceptor; and (3) 1.2 X 10 to the 19th power cm-3 donors compensated by 6.2 X 10 to the 18th power cm-3 acceptors. The calculation is based on multiple-scattering theory with the self-energy calculated self-consistently to all orders of the interaction. The results show a small but significant amount of effective band-gap narrowing.

*601,513*
**PB86-189198** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Neutron Powder Diffraction Study of the Structure of the Compound Li(sub 0.3125)La(0.5625)MoO4.**
Final rept.,
E. Lukacevic, A. Santoro, and R. S. Roth. 1986, 7p
Pub. in Solid State Ionics 18/19, p922-928 1986.

Keywords: *Crystal structure, Neutron diffraction, Reprints, *Lithium Lanthanum molybdates, Ionic conductivity, Rietveld method.

The structure of Li(0.3125)La(0.5625)MoO4 has been analyzed by the neutron powder diffraction technique and by the Rietveld method. The compound crystallizes with the symmetry of space group I41/a. The lattice parameters are a =5.3350 (1), C = 11.7584 (3) A. The structure is of scheelite type.

*601,514*
**PB86-190683** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Conductivity in the Fractionally Quantized Hall Effect.**
Final rept.,
P. M. Platzman, S. M. Girvin, and A. H. MacDonald. 1985, 4p
Pub. in Physical Review B: Solid State 32, n12 p8458-8461, 15 Dec 85.

Keywords: *Hall effect, Electron gas, Reprints, *Fractional Quantum Hall effect, *Quantum Hall effect, Electrical conductivity.

Using the recently proposed single-mode magneto-roton ansatz for the dynamic structure factor of a two-dimensional electron gas in a strong magnetic field and a weak-coupling memory-function expression for the conductivity, the authors calculate the ac and dc conductivity of such systems in the fractionally quantized Hall regime. The results suggest new experimental tests of these ideas.

*601,515*
**PB86-190691** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Calculations of Electron Inelastic Mean Free Paths from Experimental Optical Data.**
Final rept.,
C. J. Powell. 1985, 12p
Pub. in Surface and Interface Analysis 7, n6 p263-274 1985.

Keywords: *Electron scattering, *Mean free path, Copper, Magnesium, Aluminum, Aluminum oxide, Silver, Gold, Bismuth, Reprints, EV range 100-1000, KeV range 01-10.

Calculations are reported of inelastic mean free paths (IMFPs) for 100-2000 eV electrons in C, Mg, Al, Al2O3, Cu, Ag, Au, and Bi from experimental optical data. These calculations require knowledge of the momentum-transfer dependence of the differential scattering cross section; this information was taken from Penn's calculations. The calculated IMFPs agree reasonably with direct calculations and with measured electron attenuation lengths (ALs). Since accurate measurements of ALs are difficult, it is suggested that calculations of the present type are useful if the needed optical data are available. The present approach is also useful for materials (such as the transition and noble metals) for which it is not possible to make a meaningful distinction between valence-electron and core-electron excitations as required in current IMFP calculations.

*601,516*
**PB86-190709** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Energy Dependence of Electron Attenuation Lengths.**
Final rept.,
C. J. Powell. 1985, 7p
Pub. in Surface and Interface Analysis 7, n6 p256-262 1985.

Keywords: *Electron scattering, Inelastic scattering, Reprints, Energy dependence, EV range 100-1000, KeV range 01-10.

An analysis has been made of electron attenuation length data for nine materials in terms of the Bethe theory for inelastic scattering in matter. It was found that the Bethe equation adequately described the energy dependence of the data in all materials over the typical range 100-1500 eV. The Bethe equation appears to be superior to the empirical relation proposed by Wagner, Davis, and Riggs (1980).

*601,517*
**PB86-191335** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Local Properties in Orientationally Disordered Crystals with Translation-Rotation Coupling.**
Final rept.,
K. H. Michel, and J. M. Rowe. 1985, 10p
Sponsored by Institut Interuniversitaire des Sciences Nucleaires, Brussels (Belgium).
Pub. in Physical Review B: Condensed Matter 32, n9 p5827-5836, 1 Nov 85.

Keywords: Phase transformations, Abnormalities, Reprints, *Ferroelasticity.

In orientationally disordered crystals, the translation-rotation coupling affects both collective and local properties near ferroelastic phase transitions. The anomalous temperature behavior of the static mean-square displacements is investigated. The single-particle orientational distribution function in a deformable lattice is calculated and it is shown that molecular symmetry plays an essential role in addition to site symmetry. The theory is applied to a quantitative study of the alkali cyanides in the disordered phase and leads to an understanding of experimental results.

*601,518*
**PB86-192192** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Critical Behavior and Magnetic Ordering in Amorphous TbFe2.**
Final rept.,
J. J. Rhyne, and C. J. Glinka. 1984, 3p
Pub. in Jnl. of Applied Physics 55, n6 pt2A p1691-1693 Mar 84.

Keywords: Neutron scattering, Transition temperature, Reprints, *Iron terbium, *Magnetic ordering, Amorphous materials, Spin glass state.

The zero field small angle neutron scattering from amorphous TbFe2 above the magnetization-determined Tc=409 K shows a conventional Lorentzian line shape with a spin correlation length which increases to only about 135 A at and just below (T sub c). On application of a field in the range 2-12 kG at 295 K, the overall scattering at finite Q is sharply suppressed indicating an increase in the ferromagnetic component with field. The residual magnetic scattering exhibits a prolate distortion of the intensity with respect to the direction of H which demonstrates that the remaining spin clusters do not exhibit a ferromagnetic response.

*601,519*
**PB86-192507** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Chemisorption-Induced Changes in Surface Magnetism and Electronic Structure: Oxygen on Ni(110).**
Final rept.,
A. Seiler, C. S. Feigerle, J. L. Pena, R. J. Celotta, and D. T. Pierce. 1985, 3p
Sponsored by Office of Naval Research, Arlington, VA., National Science Foundation, Washington, DC., and Consejo Nacional de Ciencia y Tecnologia, Mexico City.
Pub. in Physical Review B: Condensed Matter 32, n12 p7776-7778, 15 Dec 85.

Keywords: *Surfaces, *Nickel, Chemisorption, Oxygen, Ferromagnetic materials, Reprints, *Magnetism, *Electronic structure, Band theory, Electron spin polarization, Photoemission.

The effect of oxygen chemisorption on the Ni minority-spin 3d holes-and thus the Ni magnetic moment-is measured by spin-polarized inverse photoemission. A dramatic reduction of the minority-spin 3d holes is observed, indicating a strong involvement of these states in the chemisorptive bond. This reduction can be explained by a Ni3d-O2p interaction which redistributes the density of states; no indication of a reduced exchange splitting is found. Majority-spin sp states are shown to be unchanged at coverages below the onset of nucleation and oxide formation.

*601,520*
**PB86-193208** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Spin Polarized Inverse Photoemission Studies of Surface Magnetism and Electronic Structure.**
Final rept.,
D. T. Pierce, A. Seiler, C. S. Feigerle, J. L. Pena, and R. J. Celotta. 1986, 5p
Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p617-621 1986.

Keywords: *Surfaces, Chemisorption, Nickel, Reprints, *Magnetism, *Electronic structure, Photoelectron spectroscopy, Band theory, Photoemission.

Spin polarized inverse photoelectron spectroscopy (SPIPES) is shown to be a powerful new technique to study surface and near-surface electronic structure and magnetism. The process, the information obtained, and the apparatus required in a spin polarized inverse photoemission measurement are compared to the complementary spin polarized photoemission measurement. Other SPIPES studies, such as the temperature dependent behavior of empty bands in ferromagnetic Fe, and future directions and applications of SPIPES are reviewed.

*601,521*
**PB86-193786** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Neutron Rietveld Analysis of Structural Changes in NASICON Solid Solutions Na(1+X)Zr2 Si()P(-x)O12 at Elevated Temperatures: X = 1.6 and 2.0 at 320 deg C.**
Final rept.,
J. J. Didisheim, E. Prince, and B. J. Wuensch. 1986, 15p
Grant DE-AC03-76SF00098
Sponsored by Department of Energy, Washington, DC.
Pub. in Solid State Ionics 18/19, p944-958 1986.

Keywords: *Crystal structure, Solid solutions, Sodium inorganic compounds, Zirconium inorganic compounds, Reprints, Rietveld method, Phosphates.

Neutron Rietveld analyses of the structures of NASICON solid solutions as a function of composition have been extended to 320 C for the high-conductivity composition x = 1.6 and 2.0. The transformation from the room temperature monoclinic C2/c structure to the hexagonal high temperature phase involves small atomic displacements, ranging from 0.385A for Na(2) down to shifts of only a few hundredths of an Angstrom for several framework ions. The Na(1) interstice remains fully occupied to the temperature presently examined.

*601,522*
**PB86-197357** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
**Reliability of the Isothermal Bulk Modulus Deduced from Model Equations of State.**
Final rept.,
R. G. Munro, S. Block, and G. J. Piermarini. Oct 84, 3p
Pub. in Jnl. of Applied Physics 56, n7 p2174-2176, 1 Oct 84.

Keywords: *Bulk modulus, Equations of state, Compressibility, Reprints, High pressure.

The evaluation of bulk material properties by the technique of fitting model isothermal equations of state to experimental data is discussed. Specifically, the evaluation of the isothermal bulk modulus is considered in terms of eight model equations. A sometimes serious difficulty in the application of model equations is identified, and the relationship between the error in the deduced value of the bulk modulus and the error in the measured lattice parameter or the pressure is investigated. It is found that certain of the eight equations should be avoided, and limits on the reliable application of the remaining equations are identified. Implications for the acquisition of data are discussed.

*601,523*
**PB86-199080** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Spin Polarization of Secondary Electrons in Transition Metals: Theory.**
Final rept.,
D. R. Penn, S. P. Apell, and S. M. Girvin. 15 Dec 85, 16p
Pub. in Physical Review B 32, n12 p7753-7768, 15 Dec 85.

Keywords: *Transition metals, *Iron, *Nickel, Polarization(Spin alignment), Glass, Reprints, *Electron spin polarization, Secondary electrons.

A theory of the spin polarization of the secondary electrons in transition metals and glasses is presented. In contrast to the secondary-electron intensity distribution, the spin polarization is shown to yield useful information about the electron-electron interaction. The ratio of the lifetimes of majority- to minority-spin electrons can be determined directly from the measured values of the spin polarization. The theory is applied to both Fe and Ni.

*601,524*
**PB86-200417** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Theory of Spin-Polarized Secondary Electrons in Transition Metals.**
Final rept.,
D. R. Penn, S. P. Apell, and S. M. Girvin. 29 Jul 85, 4p
Pub. in Physical Review Letters 55, n5 p518-521, 29 Jul 85.

Keywords: *Transition metals, Polarization(Spin alignment), Reprints, *Electron spin polarization, Secondary electrons, Magnetism.

It is shown that in contrast to the secondary-electron intensity distribution, the spin polarization, P(E), yields useful information about the electron-electron interaction. The ratio of lifetimes of majority- to minority-spin electrons can be determined directly from the measured values of P(E).

*601,525*
**PB86-200425** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Spin Polarized Secondary Electrons: Theory.**
Final rept.,
D. R. Penn, S. P. Apell, and S. M. Girvin. 1986, 3p
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p1041-1042 1986.

Keywords: Polarization(Spin alignment), Reprints, *Electron spin polarization, Secondary electrons, Magnetism.

It is shown that the spin polarization of the secondary electrons, P(E), yields useful information about the electron-electron interaction. The ratio of majority to minority spin lifetimes is related to the measured values of P(E).

*601,526*
**PB86-201803** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
**Preparation of Device Quality GaAs Using Plasma-Enhanced MO-CVD Technique.**
Final rept.,
K. P. Pande, and A. C. Seabaugh. 1983, 9p
Pub. in Proceedings of the Symposium on Opto-Electronics Epitaxy and Device Related Processes (3-5), San Francisco, CA., May 9-11, 1983, p201-209. Sponsored by Electrochemical Society, Inc., Pennington, NJ. Electronics Div.

Keywords: *Gallium arsenides, Semiconductors(Materials), Deposition, Epitaxy, Substrates, Plasma(Physics), *Chemical vapor deposition, Reactants.

Low-temperature (<450 C) deposition of single crystal GaAs using a new plasma-enhanced MO-CVD technique is described. In the technique, plasma is created by a dc potential and the substrate is not directly exposed to the plasma. Deposition of GaAs was achieved at extremely low plasma power (<5 W) using trimethylgallium (TMGa) and arsine (or trimethylarsenic) reactants. The resulting epitaxial films show excellent surface morphology and thickness uniformity over a large area substrate. A linear dependence of growth rate upon TMGa concentration was observed with a typical growth rate of 0.1 micrometer per minute for a TMGa flow rate of 15 cu cm per minute. Undoped films were found to be n-type with a room temperature carrier mobility in the range of 5200 sq cm/vs. Measurements on Schottky barrier devices fabricated on n/n(+) layers show uniform impurity doping profile and 55-V reverse breakdown voltage. Temperature dependence of the capacitance indicates a density of deep trapping centers as low as 6.2 x 10 to the 13th power/cu cm. Data on photoresponse of these devices are also presented.

*601,527*
**PB86-202090** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Measurements and Standards Div.
**Experimental Constraints on the Parameters Describing Unordered bcc 3He.**
Final rept.,
C. T. Van Degrift. 1983, 16p
Pub. in Proceedings of the American Institute of Physics Conference on Quantum Fluids and Solids, Sanibel Island, FL., April 11-15, 1983, p16-31.

Keywords: *Helium 3, Spin lattice relaxation, Body centered cubic lattices, Solidified gases, Nuclear magnetic resonance, Specific heat, Elastic properties, Magnetostriction, *Solid helium, Magnetism.

A wide variety of experimental results on the unordered phase of bcc (3) He are reviewed in light of recent high precision magneto-striction measurements made at NBS. Specific formulas are given for the

volume dependence of the elastic constants, Debye temperature, exchange parameters J(t) and K(p), and the Zeeman-exchange spectral density function. Some topics for further research are identified.

*601,528*
**PB86-202363** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Effect of Applied Fields on the Magnetic Order of Amorphous Tb(x)Fe(1-x) Alloys.**
Final rept.,
M. L. Spano, and J. J. Rhyne. 1986, 3p
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p300-302 1986.

Keywords: Rare earth alloys, Neutron scattering, Magnetic fields, Reprints, *Iron terbium, *Magnetic ordering, Small angle scattering, Amorphous materials, Magnetism.

The effect of applied magnetic fields on the scattering cross section and spin correlation length xi in the amorphous alloys Tb(75)Fe(25) and Tb(2)F(98) has been studied using small angle neutron scattering. In Tb(75)Fe(25), which shows effects of strong local random anisotropy, the correlation length at T/T(c) = approx 0.3 and = 0.7 is relatively independent of field up to the maximum 16 kOe used. In contrast, Tb(2)Fe(98) exhibited a sharp reduction in xi with H and a simultaneous abrupt drop in overall scattering intensity reflecting the formation of a near-infinite percolating cluster.

*601,529*
**PB86-202371** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Spin Excitations in TbNi5 by Inelastic Neutron Scattering.**
Final rept.,
D. Gignoux, and J. J. Rhyne. 1986, 2p
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p1179-1180 1986.

Keywords: Neutron scattering, Cryogenics, Single crystals, Magnons, Reprints, *Nickel terbium, Nickel intermetallics, Terbium intermetallics, Spin waves, Crystal field.

Spin waves and single-ion type magnetic excitations have been studied by inelastic neutron scattering at 4 K in a single crystal of the ferromagnetic (T(c) = 23K) hexagonal compound TbNi5 along the (q,0,0) and (O,O,q) propagation directions. One dispersive acoustic mode and two non-dispersive modes were observed. Crystal field and exchange parameters, in reasonable agreement with previous values obtained from magnetization data, were determined by a RPA pseudo-boson analysis.

*601,530*
**PB86-207529** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Effect of Surface Beveling on Carrier Profiles.**
Final rept.,
J. Albers, C. L. Wilson, and J. L. Blue. 1983, 2p
Pub. in Electrochemical Society Extended Abstracts 83-1, p641-642 1983.

Keywords: *Charge carriers, Semiconductor junctions, Electron density(Concentration), Finite element analysis, Mathematical models, Reprints, *Semiconductors.

The two-dimensional potential distribution is calculated for a beveled structure by means of finite-element techniques. The calculations are presented for several forms of the dopant distribution as well as a number of choices of the surface recombination velocity. The effects of both of these variables on the location of the electrical junction are presented with particular attention to the implications of electrical profile measurements. The principal result of the calculation is that the total depletion width goes to zero where the junction intersects the beveled surfaces.

*601,531*
**PB86-209202** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Methods of Producing Standard X-ray Diffraction Powder Patterns.**
Final rept.,
H. F. McMurdie, M. C. Morris, E. H. Evans, B. Paretzkin, and W. Wong-Ng. 1986, 4p
Pub. in Powder Diffraction 1, n1 p40-43 Mar 86.

Keywords: *X ray diffraction, *Crystal structure, Least squares method, Lattice parameters, Reprints, *Powder patterns.

Patterns useful for identification are obtained by automated diffractometer methods. The lattice constants from the experimental work are refined by least-squares methods; reflections are assigned hkl indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

*601,532*
**PB86-210010** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Investigations of Magnetic Microstructures Using Scanning Electron Microscopy with Spin Polarization Analysis.**
Final rept.,
J. Unguris, G. Hembree, R. J. Celotta, and D. T. Pierce. 1986, 2p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p1629-1630 1986.

Keywords: Polarization(Spin alignment), Electron beams, Microstructure, Reprints, *Magnetization, *Electron spin polarization, Scanning electron microscopy, Secondary electrons.

A field emission scanning electron microscope was fitted with electron spin polarization analyzers in order to image submicron magnetic microstructures. Spin polarization analysis of the emitted secondary electrons provides a direct measurement of the magnitude and direction of the magnetization in the area probed by the incident electron beam. The polarization measurement is independent of topographic contrast which is measured simultaneously. The polarization was measured using a new type of analyzer which is very compact, simple, and at least as efficient as a Mott detector. The small detector size allowed the use of multiple orthogonal detectors so that all three components of the magnetization vector could be measured. The apparatus was used to examine the domain structure of various Fe-3% Si crystals.

*601,533*
**PB86-212958** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Quasiparticle States and the Fractional Quantum Hall Effect.**
Final rept.,
A. H. MacDonald, and S. M. Girvin. 1986, 4p
Pub. in Physical Review B: Condensed Matter 33, n6 p4414-4417, 15 Mar 86.

Keywords: *Hall effect, Elementary excitations, Wave functions, Reprints, *Fractional quantum Hall effect, *Quantum Hall effect, *Quasi particles, Landau levels.

New trial wave functions are proposed for the quasiparticle states relevant to the fractional quantum Hall effect. The wave functions have the virtue that the quasiparticle energy gaps can be simply evaluated in terms of the ground-state correlation functions. In the N=0 Landau level the authors obtained (E sub g) approx = 0.114, (E sub g) approx 0.031 for nu = 1/3, nu = 1/5. In the N = 1 Landau level, for which they present the first estimates, they found (E sub g) approx = 0.059 and (E sub g) approx = 0.043 for the same fractional filling factors. The authors explain the physical origin of the unexpected difference in the nu dependence and comment on its relationship to recent experiments.

*601,534*
**PB86-212966** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Collective Excitations of Frational Hall States and Wigner Crystallization in Higher Landau Levels.**
Final rept.,
A. H. MacDonald, and S. M. Girvin. 1986, 5p
Pub. in Physical Review B: Condensed Matter 33, n6 p4009-4013, 15 Mar 86.

Keywords: *Hall effect, Reprints, *Fractional quantum Hall effect, *Quantum Hall effect, Heterostructures, Collective excitations, Landau levels.

An expression has been derived for the collective-excitation dispersion for fractional Hall states which occur in higher orbital Landau levels in terms of the electron pair-correlation function in these states. Explicit results for the n = 1 Landau level have been obtained at fractional filling factors nu = 1/2 and nu = 1/5 based on Laughlin's trial wave functions for the ground state. The results at nu = 1/3 are qualitatively different from those in the lowest Landau level and are consistent with a weak quantum Hall effect at this fraction for n = 1. The results for nu = 1/5 are similar to those in the n = 0 Landua level but the collective excitations have a higher energy. The authors associate this increase with a decrease in the fractional filling factor at which Wigner crystallization occurs. A moment sum rule is derived for pair-correlation functions in higher Landau levels.

*601,535*
**PB86-212974** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Disorder and the Fractional Quantum Hall Effect: Activation Energies and the Collapse of the Gap.**
Final rept.,
A. H. MacDonald, K. L. Liu, S. M. Girvin, and P. M. Platzman. 1986, 7p
Pub. in Physical Review B: Condensed Matter 33, n6 p4014-4020, 15 Mar 86.

Keywords: *Hall effect, Excitation, Reprints, *Fractional quantum Hall effect, *Quantum Hall effect, Heterostructures, Collective excitations.

The broadening of the collective excitations of a fractional quantum Hall state due to disorder is examined. Because of the absence of screening at long wavelength in this regime, the authors believe that the broadening depends mostly on the ionized impurity contribution to the disorder potential. The broadening of the collective excitation spectrum reduces the minimum excitation energy and eventually the gap required for the occurrence of the fractional quantum Hall effect collapses. The authors present some results on the necessary conditions for the gap to remain finite. These depend on some exact sum rules for three-point correlation functions of isotropic states constructed entirely within the lowest Landau level. Finally the relationship between their results and the activation energies seen in the magnetotransport coefficients is discussed.

*601,536*
**PB86-214699** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**New X-ray Powder Diffraction Patterns from the JCPDS Associateship.**
Final rept.,
H. F. McMurdie, M. C. Morris, E. H. Evans, B. Paretzkin, and W. Wong-Ng. Mar 86, 21p
Pub. in Powder Diffraction 1, n1 p77-99 Mar 86.

Keywords: *X ray diffraction, *Crystal structure, Least squares method, Reprints, *Powder patterns.

The following new or updated patterns are submitted by the JCPDS Associateship at the National Bureau of Standards. The patterns are a continuation of the series of publications in NBS Circular 539 and NBS Monograph 25. The data for each phase apply to the specific sample described. A sample was mixed with 1 or 2 internal standards, traditionally silicon (SRM 640a), silver (a(0)=4.08651 A), tungsten (a(0)=3.16524 A), or fluorophlogophite (SRM 675). Data were measured with a computer controlled diffractometer, and computer programs were used to locate peak positions as well as to perform variable indexing and least squares cell refinement. Intensities were measured as peak heights above background, and were read manually from strip charts. Details of this procedure are given in another publication.

*601,537*
**PB86-229671** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
**Effect of Fluid Flow Due to the Crystal-Melt Density Change on the Growth of a Parabolic Isothermal Dendrite.**
Final rept.,
G. B. McFadden, and S. R. Coriell. 1986, 6p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Crystal Growth 74, p507-512 1986.

Keywords: *Dendritic crystals, *Crystal growth, Supercooling, Fluid flow, Volume, Reprints.

The Ivantsov analysis of an isolated isothermal dendrite (with zero surface tension) growing into a supercooled liquid is extended to include the effects of the fluid flow due to volume contraction or expansion upon solidification. For an axisymmetric paraboloidal dendrite an analytic solution to the Navier-Stokes equations is obtained. The magnitude of the flow is proportional to the relative density change epsilon and the flow becomes negligible far from the surface of the dendrite. The temperature field consistent with the flow can also be found explicitly. The well-known expression that relates the dimensionless supercooling to the Peclet number in the absence of fluid flow is modified for nonzero epsilon, but the effect is of order epsilon and hence is seen to be minor for most values of epsilon and dimensionless supercooling that occur in practice.

*601,538*
**PB86-230380** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Semiconductor Measurement Technology: Analytic Analysis of Ellipsometric Errors.**
Final rept.,
D. Chandler-Horowitz. May 86, 39p NBS/SP-400/78
Also available from Supt. of Docs as SN003-003-02733-2. Library of Congress catalog card no. 86-600541.

Keywords: *Polarimetry, Silicon, Oxides, Substrates, Thickness, Errors, Films, Computer programs, Fortran, *Ellipsometry, Refractive index, Uncertainty, Semiconductor materials.

A FORTRAN program was developed that calculates the ellipsometric measurement uncertainties for two models of a surface. The first is the simple bare isotropic substrate model. The second is the isotropic nonabsorbing film-substrate model. It is assumed that the sample to be measured ellipsometrically can be best described by one of these two models.

*601,539*
**PB86-231123** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
**Local Structure at Mn Sites in Icosahedral Mn-Al Quasicrystals.**
Final rept.,
E. A. Stern, Y. Ma, and C. E. Bouldin. 1985, 4p
Pub. in Physical Review Letters 55, n20 p2172-2175, 11 Nov 85.

Keywords: X ray absorption, Reprints, *Quasicrystalline materials, *Aluminum manganese, Amorphous materials, Aluminum intermetallics, Manganese intermetallics.

Extended x-ray-absorption fine-structure measurements have been made at the Mn K edge of quasicrystalline and crystalline forms of an Al6Mn alloy. Two different quasicrystalline Mn sites are discerned to be populated in the ratio of tau, the golden mean, within experimental error. The more populous site is similar to that in the crystal but with bond-angle distortions and elimination of an unusually short Al-Mn bond, while the other site has additional bond-stretching distortions. The measurements, together with density measurements, indicate that the volume per Mn site is independent of the type of site.

*601,540*
**PB86-238391** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Disclinations.**
Final rept.,
R. deWit. 1986, 3p
Pub. in Encyclopedia of Materials Science and Engineering, v2 p1208-1210 1986.

Keywords: *Defects(Materials), Magnetic domains, Liquid crystals, Reprints, *Disclinations, Dislocations.

The concept of the disclination is defined and briefly described.

*601,541*
**PB86-238433** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
**Effect of Bevel Angle and Number of Points on Spreading Resistance Data-Analysis.**
Final rept.,
J. Albers, C. L. Wilson, and J. L. Blue. 1984, 1p
Pub. in Jnl. of the Electrochemical Society 131, n8 p319 1984.

Keywords: Mathematical models, Charge carriers, Angles(Geometry), Algorithms, Reprints, *Semiconductors, *Spreading resistance, Bevels.

The semiconductor equations are used to obtain the carrier profile along a beveled structure. The spreading resistance is calculated on a scale much finer than the present experimental resolution of the technique. Spreading resistance algorithms are used on data spaced at the present experimental resolution. The difference between atomic and carrier densities along the bevel and the errors inherent in finite-layer algorithms are investigated. This is meant to provide insight into limitations of spreading resistance due to these sources.

*601,542*
**PB86-241361** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**CO Chemisorption on Ni(110): Effect on Surface Magnetism.**
Final rept.,
C. S. Feigerle, A. Seiler, J. L. Pena, R. J. Celotta, and D. T. Pierce. 1986, 4p
Prepared in cooperation with Consejo Nacional de Ciencia y Tecnologia, Mexico City. Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in Physical Review Letters 56, n20 p2207-2210, 19 May 86.

Keywords: *Carbon monoxide, *Chemisorption, *Nickel, Surfaces, Reprints, *Magnetism, *Electronic structure, Electron spin polarization, Photoemission.

The effect of CO chemisorption on the surface magnetism and unfilled electronic structure of Ni(110) is investigated by spin-polarized inverse-photoemission spectroscopy. A saturation in the reduction of the unfilled minority-spin d density of states is observed near 0.5-monolayer CO coverage and attributed to a reduction in the Ni-atom magnetic moments. Transitions into the CO (pi star) band are also observed with an intensity that increases nearly linearly with coverage. No transference of spin polarization from the Ni substrate to the CO (pi star) is found.

*601,543*
**PB87-105037** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.
**Contribution to the Theory of Surface Energy Minimizing Shapes.**
Final rept.,
J. W. Cahn, and J. E. Taylor. 1984, 4p
Pub. in Scripta Metallurgica 18, n10 p1117-1120 1984.

Keywords: *Surfaces, Free energy, Optimization, Reprints, Crystal surfaces, Flat surfaces.

A conjecture about the equilibrated shapes of facetted surfaces, which J. W. Cahn and others have believed true, is disproved by a counterexample.

*601,544*
**PB87-105888** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**CITATION CLASSIC In Current Contents/Physical, Chemical and Earth Sciences.**
Final rept.,
D. R. Penn. 1985, 2p
Pub. in Current Contents/Physical, Chemical and Earth Sciences 25, n6 p20-21 1985.

Keywords: Dielectric properties, Reprints, *Semiconductors, Penn model.

A simple model for a semiconductor is proposed. The model is isotropic and the electrons occupy a sphere in a momentum space and are surrounded by an isotropic energy gap. The wave-number dependent dielectric function is calculated.

*601,545*
**PB87-106142** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Ferromagnetic Resonance at 9.55 and 23.9 GHz in the Weak Ferromagnet Ni3Al.**
Final rept.,
B. Heinrich, J. F. Cochran, K. Myrtle, G. Lonzarich, and R. B. Goldfarb. 1986, 2p
Pub. in Jnl. of Magnetism and Magnetic Materials 54-57, p1011-1012 1986.

Keywords: Ferromagnetic materials, Cryogenics, Reprints, *Aluminum nickel, *Ferromagnetic resonance, Nickel intermetallics, Aluminum intermetallics.

Ferromagnetic resonance at microwave frequencies of 9.55 and 23.9 GHz has been measured in the archetypal weak itinerant ferromagnet Ni3Al in the temperature range 4-60 K. The observed FMR lines exhibited a strong Dysonian asymmetry and were well described over the whole temperature range by Maxwell's equations that included eddy currents, and by the Landau-Lifshitz (L-L) equation of motion including either Gilbert or L-L damping terms.

*601,546*
**PB87-107330** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Rapid X-ray Topographic Examination of GaAs Crystals.**
Final rept.,
R. A. Forman, M. I. Bell, and S. Mayo. 1985, 7p
Pub. in Proceedings of Conference on Defect Recognition and Image Processing in III-V Compounds, Montepellier (France) July 2-4, 1985, p56-62.

Keywords: *Gallium arsenides, Crystal defects, Czochralski method, Crystal growth, *X ray topography, *Dislocations.

The design of a low-cost, high-throughput x-ray topography system is described, and its use in the examination of commercial GaAs wafers is demonstrated. Double-crystal reflection (Bragg) topographs are obtained in two minutes and transmission (Laue) topographs in fifteen minutes, using copper K(alpha) radiation from a conventional 1 KW fine-focus laboratory x-ray source. Reflection topographs of typical GaAs wafers using selected diffracting planes are presented, and their relative sensitivity to various defects are discussed. In crystals grown by the liquid encapsulated Czochralski method, transmission topographs using the (220) planes display the well-known large-scale dislocation patterns produced by relaxation of thermoelastic stress.

*601,547*
**PB87-107371** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
**Epitaxial Growth and Some Properties of Samarium Crystals on Tungsten.**
Final rept.,
A. Ciszewski, and A. J. Melmed. 1984, 4p
Pub. in J. Phys., Colloq. C9, p39-42 1984.

Keywords: *Samarium, Vapor plating, Tungsten, Reprints, *Epitaxial growth, Low energy electron diffraction.

Samarium epitaxial crystalline layers have been grown by vapor deposition onto either tungsten field-electron emitters or a single macro-crystal, (011)-oriented tungsten low-energy-electron diffraction specimen. Optimum growth occurred for substrate temperatures in the range 650-750 K. The epitaxial relationship most commonly observed was (0001)Sm // (011)W with (11-20)Sm // (001)W. The surface lattice constant of Sm(0001) appears to be a few percent larger than the bulk value.

*601,548*
**PB87-109864** PC **A05**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Journal of Research of the National Bureau of Standards, Volume 91, Number 4, July-August 1986.**
Aug 86, 84p
See also PB87-109872 through PB87-109898, and PB87-100186. Also available from Supt. of Docs as SN703-027-00011-3.

Keywords: *Research, Ophthalmology, Calibrating, Electron tunneling, Measurement, Radiation doses, Electron dosimetry.

Contents: Calibration of Beta-Particle Ophthalmic Applicators at the National Bureau of Standards; Room Temperature Gold-Vacuum-Gold Tunneling Experiments; Conference on Precision Electromagnetic Measurements.

*601,549*
**PB87-109880**
(Order as PB87-109864, PC **A05**/MF **A01**)
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Room Temperature Gold-Vacuum-Gold Tunneling Experiments,**
E. C. Teague. 24 Apr 86, 45p
Included in Jnl. of Research of the National Bureau of Standards, v91 n4 p171-215 Jul-Aug 86.

Keywords: *Electron tunneling, Work functions, Gold, Vibration isolators, Theses, Scanning tunneling microscopy.

An experiment has been completed which demonstrated quantum mechanical tunneling of electrons between two gold electrodes separated in vacuum. The tunneling current between the gold electrodes has been measured, for fixed voltages of 0.1 and 0.01 volts, as the electrode spacing was varied from a distance of approximately 2.0 nm down to a point where the electrodes touched. Current changes of over five orders of magnitude were found for electrode spacing changes of approximately 1.2 nm. For the first time, these data enable one to deduce the work function of the electrodes in a tunneling experiment from experimental parameters independent of the tunneling device. Also obtained were current-voltage characteristics for fixed electrode spacings in the direct tunneling region where electrode spacings were less than 2.0 nm.

*601,550*
**PB87-119731** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Equilibrium and Diffusion in Stressed Solid Solutions with Defects.**
Final rept.,
F. Larche, and J. W. Cahn. 1986, 27p
Pub. in Solute-Defect Interaction: Theory and Experiment, p1-27 1986.

Keywords: *Diffusion, Solid solutions, Stresses, Thermodynamics, Creep properties, Reprints, Dislocations.

The recent developments in the thermodynamics of stressed solids with mobile components and defects are reviewed. Stress affects solubility and phase equilibria. The effect of stress on the composition field is equivalent to an additional elastic compliance and many problems of the equilibrium redistribution of mobile components in a stress field can be formulated as a purely elastic problem using what we call open-system elastic coefficients. The stress fields generated by an inhomogeneous composition field are an implicit part of the formulation. Diffusion in either an applied or self-generated stress field is considered. The concept of open-system elastic coefficients is presented. It greatly simplifies the equations of the thermodynamics of stressed solid solutions. It is used to study the interactions of dislocations and composition in isotropic and cubic crystals. The vacancies equilibrium is reviewed, in the interior and near the surfaces of a solid. The effects of these thermodynamics results on the diffusion equations and on their boundary conditions are examined. Problems connected with diffusional creep are discussed.

*601,551*
**PB87-119756** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**Standard X-Ray Diffraction Powder Patterns from the JCPDS Research Associateship.**
Final rept.,
H. F. McMurdie, M. C. Morris, E. H. Evans, B. Paretzkin, and W. Wong-Ng. 1986, 14p
Sponsored by JCPDS-International Centre for Diffraction Data, Swarthmore, PA.
Pub. in Powder Diffraction 1, n2 p64-77 Jun 86.

Keywords: *Crystal structure, *X-ray diffraction, *Standards, Reprints, *Powder patterns.

Standard x-ray powder diffraction patterns are presented for 20 substances. These patterns, useful for identification, were obtained by automated diffractometer methods. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned hkl indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

*601,552*
**PB87-119814** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Electron Tunneling into Superconducting Filaments: Depth Profiling the Energy Gap of NbTi Filaments from Magnet Wires.**
Final rept.,
J. Moreland, J. W. Ekin, and L. F. Goodrich. 1986, 8p
Sponsored by National Research Council, Washington, DC., and Department of Energy, Washington, DC.
Pub. in Advances in Cryogenic Engineering Materials 32, p1101-1108 1986.

Keywords: *Superconductors, *Electron tunneling, Reprints, *Niobium titanium, *Energy gaps (Solid state), Tunneling spectroscopy.

Squeezable electron tunneling (SET) junctions consisting of superconducting NbTi filaments (extracted from magnet wires) and sputtered Nb thin-film counter electrodes were used to determine the energy gap at the surface of the filaments. The current versus voltage curves of junctions immersed in liquid helium at 4 K were measured for a series of filaments taken from the same wire. Each filament had been etched to remove a surface layer of varying thickness so that the energy gap could be determined as a function of depth into the surface of an 'average' filament. It was found that some manufacturing processes yield filaments having surface layers with reduced energy gaps of 0.4 meV compared to measured interior bulk values ranging from 1.2 to 1.3 meV.

*601,553*
**PB87-125753** PC **A06**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Electromechanical Properties of Superconductors for DOE (Department of Energy) Fusion Applications,**
J. W. Ekin, J. Moreland, and J. C. Brauch. Mar 86, 112p NBSIR-86/3044
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Keywords: *Superconductors, Superconducting magnets, Critical field, Strains, Electron tunneling, Niobium intermetallics, Tin intermetallics, *Fusion reactors, *Niobium tin, Critical current, Lead molybdenum sulfides.

Contents:
- Uniaxial strain-effect characterization of new high-field experimental superconductors;
- High-field uniaxial strain effect characterization of candidate Nb3Sn superconductors for fusion applications--Internal tin, jelly roll, bronze process;
- Construction and initial testing of a transverse-stress-effect apparatus;
- Thermal contraction of several candidate sheathing and strengthening materials for superconductors;
- Electron tunneling into superconducting filaments using mechanically adjustable barriers;
- Appendix A--Effect of stainless steel reinforcement on the critical current versus strain characteristic of multifilamentary Nb3Sn superconductors;
- Appendix B--Further investigations of the solid-liquid reaction and high-field critical current density in liquid-infiltrated Nb-Sn superconductors;
- Appendix C:
- Japan trip report, December 5-14, 1984.

*601,554*
**PB87-128013** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Thermal Fluctuations in Interfaces: From Fluid-Fluid Interfaces to Small-Angle Grain Boundaries.**
Final rept.,
C. Rottman. 1986, 10p
Pub. in Materials Science and Engineering 81, p553-562 1986.

Keywords: *Grain boundaries, *Interfaces, Reprints, Capillary waves, Dislocations.

In the tutorial overview, thermal fluctuations in several interfaces, especially small-angle grain boundaries, are considered. The emphasis is placed on large-distance fluctuations, which are important in characterizing equilibrium interfacial phases. Capillary wave fluctuations prove to be crucial in fluid-fluid interfaces and in the high temperature solidfluid interfacial phase. In small-angle grain boundaries the energy cost of simply allowing waves in the dislocation configurations which make up the boundary is much more than that of the corresponding capillary waves in fluid-fluid or solid-fluid interfaces. The introduction of dislocation loops with a different Burgers vector may be an important fluctuation in high temperature small-angle grain boundaries. Possible experimental consequences are presented.

*601,555*
**PB87-128104** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Impurity Bands and Band Tailing in n-Type GaAs.**
Final rept.,
J. R. Lowney. 1986, 6p
Pub. in Jnl. of Applied Physics 60, n8 p2854-2859, 15 Oct 86.

Keywords: *Gallium arsenicles, *Energy bands, Band structure of solids, Impurities, Reprints, N type semiconductors, Density of states.

The density of states of the valence and conduction bands of n-type GaAs has been calculated for a donor density of 10 to the 17th power/cc at 300 and 20 K. Both the donor-carrier and carrier-carrier interactions have been included. Band tails appear on both bands and the energy gap is narrowed. Calculations were also performed for a donor density of 10 to the 15th power/cc at 300 and 20 K. These results show the formation of an impurity band at 20 K, whereas a band tail exists at 300 K.

*601,556*
**PB87-128344** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**High-Field Flux Pinning and the Strain Scaling Law.**
Final rept.,
J. W. Ekin. 1985, 5p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Proceedings of International Symposium on Flux Pinning and Electromagnetic Properties in Superconductors, Fukuoka (Japan), November 11-15, 1985, p267-271.

Keywords: *Superconductors, *Strains, Critical field, Niobium intermetallics, Tin intermetallics, *Flux pinning, Niobium tin, Scaling laws.

The effects of strain on flux pinning in superconductors are discussed. Significant differences between the strain scaling law, temperature scaling law, and the flux-line-shearing model of Kramer are demonstrated. The strain scaling law is more general than current flux-pinning models, and as such, it may serve as a guide to future work on flux pinning theory. Flux-pinning measurements at fields up to 24 T have been made on a series of high-quality Nb3Sn samples with third (and fourth) element additions. The data show that the usual extrapolation procedures for determining the bulk-average upper critical field in Nb3Sn lead to significant errors when additives such as Ti, Ta, Ga, and Hf are present.

*601,557*
**PB87-128351** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Relationships between Mechanical and Magnetoelectric Properties of Oxygen-Free Copper at 4 K.**
Final rept.,
F. R. Fickett, and T. E. Capobianco. 1986, 7p
Pub. in Advances in Cryogenic Engineering Materials 32, p421-427 1986.

Keywords: *Copper, *Electrical resistivity, *Magnetoresistivity, Superconductors, Stabilization, Cryogenics, Reprints.

Commercially pure, oxygen-free copper is the material of choice for nearly all superconductor stabilization. Straining relatively pure copper at 4 K can result in significant increases in the residual resistivity and, thus, a decreased ability of the copper to stabilize the super-

conductor. In the paper the authors quantify the effect of strain on the resistivity and magnetoresistivity of a number of oxygen-free coppers from various sources and in various tempers. In addition, the low temperature stress-strain behavior of these materials and its correlation with room temperature data and the residual resistivity ratio (RRR) prior to straining is discussed. An apparatus developed for testing of mechanical properties of relatively small wire samples at low temperatures is described.

*601,558*
**PB87-130050** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Neutron Diffraction Studies of the Icosahedral Phase of Al-Mn Alloys.**
Final rept.,
B. Mozer, J. W. Cahn, D. Gratias, and D. Shechtman. 1986, 10p
Pub. in Jnl. de Physique 47, n7 pC3-351-C3-360 Jul 86.

Keywords: *Neutron diffraction, *Crystal structure, Crystallography, Grain structure, Crystal lattices, Concentration(Composition), Reprints, *Aluminum manganese alloys, Icosahedral phase, Diffraction analysis.

Powder neutron diffraction studies were performed on three icosahedral alloys of the aluminum manganese system containing 27, 30, and 34 weight percent manganese. All peaks were found at the angles consistent with the icosahedral indexing with a six-dimensional cubic lattice parameter of approximately 0.65 nm that decreased with increasing Mn content. The relative intensities differ significantly from those found for X-rays. The intensities are not consistent with a quasilattice consisting of the 3-dimensional Penrose tiling with a .46 nm edge length along the 5-fold axis. It is consistent with a 1.0 nm edge along the 3-fold axis quasilattice node separation.

*601,559*
**PB87-131801** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Tetrahedron Treatment of the FCC Lattice.**
Final rept.,
R. Kikuchi, and J. L. Murray. 1985, 38p
Pub. in CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry 9, n4 p311-348 1985.

Keywords: *Order disorder transformations, *Phase diagrams, Face centered cubic lattices, Computer programs, Reprints, *FCC lattices, Binary alloys, Copper gold.

A computer program for calculating the disorder-order phase diagrams of FCC-based binary alloys is presented. The cluster variation method is used, with the tetrahedron as the basic cluster. Ordered phases are the Cu3Au type (L1 sub 2) and the CuAu type (L1 sub 0). Energy parameters are independent of temperature and composition, and include the many-body effect with a tetrahedron. A detailed explanation of the computer program is presented in the main body of the paper. Three example calculations are shown.

*601,560*
**PB87-134995** Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**Stacking Fault Tetrahedron.**
Final rept.,
G. Kalonji, and J. W. Cahn. 1986, 9p
Pub. in Philosophical Magazine A-Defects and Mechanical Properties 53, n4 p521-529 1986.

Keywords: *Crystal defects, *Stacking fault, *Tetrahedrons, Crystallography, Reprints.

Based on symmetry arguments the authors conclude that what is called a stacking fault tetrahedron is really a self-inclusion in which a portion of the same crystal is shifted by 1/4 (111) relative to the enclosing matrix. The included crystal has fewer atoms than would have been required to fill the hole in the matrix crystal with perfect material, and this is a way of accommodating clusters of vacancies. Symmetry shows that for this shift the energy is at an extremum and that the form of the inclusion must conform to the point group 4 bar 3m (tetrahedral). Compared to the usual description this is a simpler model and even the unrelaxed version has lower energy for small sizes. For intermediate sizes it would relax to the same description as the relaxed version of the defect as conventionally described, and at large sizes the stacking fault tetrahedra are unstable with respect to Frank loops.

*601,561*
**PB87-135182** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Electronic Properties, Superconductivity and Stability of the Zr-Rh Alloys.**
Final rept.,
R. Kuentzler, and R. M. Waterstrat. 1985, 8p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Solid State Communications 54, n6 p517-524 1985.

Keywords: *Superconductors, Band structure of solids, Phase diagrams, Reprints, *Rhodium zirconium, Electronic specific heat, Magnetic susceptibility.

Experimental information on the electronic properties of ordered Zr-Rh alloys is presented through low temperature specific heat and magnetic susceptibility measurements. In general, a low density of states at the Fermi level is deduced and this is explained by a split band regime consistent with the known DOS calculations for the type of ordered structures considered. The existence of a split band is considered as typical of stable ordered structures. Zr2Rh, which is a superconductor with T(c) = 11.2 K, possesses a very high electronic specific heat coefficient. It is suggested that the high gamma value is associated with a decrease of stability of the ordered structure and increased ability to form amorphous alloys when the concentration of Zr increases.

*601,562*
**PB87-135190** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Thermal Fluctuations in Low-Angle Grain Boundaries.**
Final rept.,
C. Rottman. 1986, 6p
Pub. in Acta Metallurgica 34, n12 p2465-2470 1986.

Keywords: *Grain boundaries, Dislocations, Entropy, Crystallography, Reprints, Thermal fluctuations.

Thermal fluctuations in a low-angle, symmetric tilt boundary composed of a series of dislocations of identical Burgers vectors are studied. At zero temperature the grain boundary is composed of equally spaced, coplanar, straight dislocations. At nonzero temperatures the dislocations are allowed to fluctuate a small distance both in and out of the zero-temperature plane. The energy of a sinusoidal fluctuation is shown to be linear in wave number for oscillations both parallel and perpendicular to the dislocations. These excitations give rise to a decrease in the / theta ln/theta// term of the grain-boundary free energy, where theta is the angle of misorientation between the two grains, linearly proportional to temperature. The grain boundary considered here, with these fluctuations, is argued to be smooth, not rough.

*601,563*
**PB87-136610** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
**High Pressure Crystallography.**
Final rept.,
S. Block, and G. Piermarini. 1983, 3p
Pub. in Crystallography in North America, Ch14, p265-267 1983.

Keywords: *Crystallography, *High pressure.

No abstract available.

*601,564*
**PB87-140174** PC **A03**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
**Nondestructive Evaluation Activities in the Semiconductor Materials and Processes Division,**
R. D. Larrabee, and M. I. Bell. Dec 86, 33p NBSIR-86/3495

Keywords: Electrical resistivity, Semiconductor devices, Line width, Raman spectroscopy, Photoluminescence, *Semiconductor materials, Fourier transform infrared spectroscopy, Deep level transient spectroscopy, Carrier lifetime, Ellipsometry, X ray topography.

This is the first in a planned series of annual reports describing the nondestructive evaluation and measurement development activities of the National Bureau of Standards in the area of semiconductor materials and devices. Present activities include production and certification of standard reference materials, development of new measurement techniques, and coordination of interlaboratory experiments and other activities of voluntary standards organizations.

*601,565*
**PB87-140414** PC **A04**/MF **A01**
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Crystal Data: Version 1.0 Database Specifications.**
Final rept.,
J. K. Stalick, and A. D. Mighell. Nov 86, 75p NBS/TN-1229
Also available from Supt. of Docs as SN003-003-02781-2.

Keywords: *Crystal structure, Crystallography, Information retrieval, Minerals, Metals, Organometallic compounds, Tables(Data), Physical properties, Solid state physics, *Crystal data database, National Bureau of Standards.

The NBS Crystal Data database is a file of crystallographic and chemical data covering a broad spectrum of solid-state materials: inorganics, minerals, metals, intermetallics, organics, and organometallics. To be included in the database the unit-cell parameters of a material must be known. With the aid of computer programs, the data were evaluated by the Editors for reasonableness and self-consistency, and errors or possible errors are noted. The data items have been formatted in a standard way to permit searches. Each entry in the database contains unit-cell data (initial cell, convential Crystal Data cell, and reduced cell), space group or diffraction aspect, formula units per cell, observed and calculated densities, literature reference, chemical or mineral name, chemical formula, empirical formula, and an indication of the extent to which the atomic positional parameters have been determined. In addition to identification of unknowns by lattice-matching techniques, the large size of the database along with the combination of crystallographic, chemical and physical information make this file a valuable resource for all of solid-state science. Detailed format and content specifications are given.

## Structural Mechanics

*601,566*
**PB86-160975** Not available NTIS
National Bureau of Standards (IMSE), Boulder, CO. Fracture and Deformation Div.
**Elastic-Plastic Fracture Toughness Tests with Single-Edge Notched Bend Specimens.**
Final rept.,
T. L. Anderson, H. I. McHenry, and M. G. Dawes. 1985, 20p
Sponsored by Minerals Management Service, Washington, DC.
Pub. in Proceedings of the Symposium on Elastic-Plastic Fracture Test Methods: The User's Experience, Louisville, KY., April 20-22, 1983, ASTM (American Society for Testing and Materials) Special Technical Publication 856, p210-229 1985.

Keywords: *Fracture tests, *Toughness, Fracture strength, Mechanical properties, Tests, Crack propagation, Notch tests, Fracture properties, Structural steels.

Fracture toughness tests have been performed on five geometries of single-edge notched bend (SENB) specimens machined from a 25.4-mm (1.0-in.) thick plate of ABS Grade EH36 steel, a normalized carbon-manganese steel. Critical values of the J integral and the crack-tip opening displacement (CTOD) were measured as a function of temperature. Test temperatures, which ranged from -196 to 25 degrees C, covered the entire ductile-to-brittle transition range. On the upper shelf, critical values of J and CTOD at the onset of stable crack growth were insensitive to specimen geometry. However, in the ductile-to-brittle transition region, where fracture occurred by unstable cleavage, fracture toughness decreased with increasing specimen thickness and crack length. The effect of geometry on fracture toughness in the transition region is attributed to changes in crack-tip region constraint with geometry.

*601,567*
**PB86-196649** Not available NTIS
National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.
**Distribution of Stress in a Craze of the Tip of a Uniformly Extending Crack.**
Final rept.,
E. Passaglia. 1984, 7p
Pub. in Polymer 25, n12 p1727-1733 1984.

Keywords: *Crazing, *Cracks, *Stress concentration, Displacement, Stresses, Reprints.

A model of a craze at the tip of a uniformly extending crack is developed which permits the calculation of the stress distribution in the craze. In accord with experimental observations by Kramer (11) the craze is modelled as a collection of independent fibrils that draw from the substrate by a process akin to the drawing of textile fibers with necking. Except at the very tip of the craze where complex yielding type phenomena occur, the stress in the craze is taken to correspond to the drawing stress. The craze stress is treated as the cohesive crack closing stresses in the Barenblatt treatment of crack tips. The principal fact used in the development is that the drawing stress depends upon the rate of draw and hence upon the slope of the craze displacement. This leads to a non-linear integral equation for the craze stress. Using an empirical relation between drawing stress and rate of draw, the equation is solved for the stress distribution in the craze by numerical methods. The distribution shows peaks at the craze tip and at the crack tip as observed in some experiments. The magnitude of the peaks depends upon the material parameters used. For certain values of these parameters, the constant stress Dugdale model yields a good approximation to the displacement profile.

*601,568*
**PB86-201019** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Institute for Materials Science and Engineering.
**Dislocation Shielding of Cracks and the Fracture Criterion.**
Final rept.,
R. Thomson. 1983, 6p
Sponsored by Chinese Society of Theoretical and Applied Mechanics, Beijing, and Chinese Aeronautics and Astronautics Society, Beijing.
Pub. in Proceedings of ICF International Symposium on Fracture Mechanics, Beijing, China, November 22-25, 1983, p1019-1024 1984.

Keywords: *Fractures(Materials), *Cracks, Dislocations(Materials), Shielding, Theories, *Fracture(Mechanics).

A theory of fracture for review with application to moving cracks in two applications. The results show a brittle break-away effect at a critical stress intensity.

*601,569*
**PB86-245743** PC **A06**/MF **A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Fracture Mechanics Characterization of Crack Arrest and Reinitiation in Two Unconventional Specimens,**
T. Teramoto, D. T. Read, and R. B. King. Jun 86, 120p NBSIR-85/3034
Sponsored by Office of Naval Research, Arlington, VA., and David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.

Keywords: *Crack propagation, *Fracturing, Fracture properties, Steel structures, Crack arrest.

A simple elastic-plastic-fracture-mechanics-based model of crack propagation, arrest, re-initiation, and propagation is described. This model requires much less computing resources than dynamic, elastic-plastic finite element calculations, and allows estimates of applied J-integral, load, and crack mouth opening displacement during initial rapid crack propagation, re-initiation and repropagation. A comparison of this new model to other available models and to experimental results indicates that it can successfully reproduce the essential features of the behavior of specimens containing propagating cracks.

*601,570*
**PB87-104758** PC **A04**/MF **A01**
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Cycle-Counting Methods for Fatigue Analysis with Random Load Histories: A Fortran User's Guide,**
Y. W. Cheng, and J. J. Broz. Aug 86, 52p NBSIR-86/3055
Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Fatigue(Materials), *Counting, FORTRAN, Computer programs, Loads(Forces).

Rainflow and mean crossing-range methods are used in counting the stress ranges and cycles of a random load history. Each method is defined and then applied to a simple random load history example. Fortran IV computer programs were written to make analysis of long random load histories possible. The stress ranges and cycles obtained by these programs have been used for fatigue crack growth analysis under sea-wave loading.

*601,571*
**PB87-117958** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Acoustic Refraction of Off-Axis Shear Horizontal Waves in Slightly Anisotropic Plates.**
Final rept.,
A. V. Clark, and P. P. Delsanto. 1986, 6p
Prepared in cooperation with Naval Research Lab., Washington, DC.
Pub. in Ultrasonics, p25-30 Jan 86.

Keywords: *Acoustic refraction, *Anisotropic plates, *Stress analysis, Anisotropy, Reprints, Acoustical birefringence.

Several techniques have recently been proposed to perform acoustic birefringence measurements, using off-axis SH-waves, in order to determine stresses in slightly anisotropic materials. These techniques tacitly assume that refraction effects, due to inhomogeneous stress distributions and/or local variations in material properties are negligible. In the paper the authors investigate the conditions under which this assumption is valid.

*601,572*
**PB87-118550** Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
**Fracture Mechanics.**
Final rept.,
H. I. McHenry. 1985, 6p
Pub. in ASTM (American Society for Testing and Materials) Standardization News, p38-43 Nov 85.

Keywords: Standards, Fractography, Reprints, *Fracture(Mechanics).

The article reviews some of the early ideas that have shaped fracture mechanics, some notable failures that have spurred its development, some ways it is currently used to help prevent fracture, and some work underway in ASTM Committee E-24 to extend its usefulness.

## General

*601,573*
**AD-P002 450/5** PC **A02**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD.
**Laser Cooled 9Be+ Accurate Clock,**
J. J. Bollinger, W. M. Itano, and D. J. Wineland. 1983, 5p
Pub. in the Proceedings of the Annual Symposium on Frequency Control (37th), 1-3 Jun 83, Marriott Hotel, Philadelphia, PA., AD-A136 673, p37-41.

Keywords: *Frequency standards, *Beryllium, *Clocks, Lasers, Cooling, Ions, Accuracy, Measurement, Clouds, Frequency, Doppler effect, Component Reports.

The use of laser cooled stored ions in an atomic frequency standard has the potential of very high accuracy because Doppler effects are greatly suppressed. A clock based on the ground-state hyperfine transition in 201Hg+ has potential accuracy and stability exceeding 1 part in 1015. However, laser cooled 9Be+ ions are experimentally easier to obtain. Therefore a 9Be+ based frequency standard is investigated in order to study the generic problems of laser cooled stored ion frequency standards.

*601,574*
**AD-P002 453/9** PC **A02**/MF **A01**
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**National and International Time and Frequency Comparisons,**
D. W. Allan. 1983, 6p
Pub. in the Proceedings of the Annual Symposium on Frequency Control (37th), 1-3 Jun 83, Marriott Hotel, Philadelphia, PA., AD-A136 673, p55-60.

Keywords: *Frequency standards, *Atomic clocks, Comparison, Time, Global positioning system, Measurement, Clocks, Accuracy, Methodology, Component Reports.

The advent of satellite time and frequency comparison techniques has provided the opportunity for measuring the time and frequency difference between remote clocks with greatly improved accuracies. The paper will give a brief review of various remote clock comparison techniques; in particular the Global Positioning System (GPS) will be highlighted.

*601,575*
**DE83010760** PC **A02**/MF **A01**
Argonne National Lab., IL.
**Overview of Research at NBS Using Synchrotron Radiation at SURF-II.**
D. L. Ederer, R. P. Madden, A. C. Parr, G. Rakowsky, and E. B. Saloman. 1982, 6p CONF-821123-40
Contract W-31-109-ENG-38
Conference on the application of accelerators in research and industry, Denton, TX, USA, 8 Nov 1982, Microfiche only, copy does not permit paper copy reproduction.
Pub. in IEEE Trans. Nucl. Science NS-30, n2 p1020-1025 April 83.

Keywords: *Synchrotron Radiation, Ultraviolet Radiation, Monochromatic Radiation, Research Programs, Molecular Structure, Solid State Physics, Atomic Physics, ERDA/430303, ERDA/640300, ERDA/656000.

The National Bureau of Standards (NBS) Synchrotron Ultraviolet Radiation Facility (SURF-II) is used in conjunction with several high throughput monochromators to study the interaction of vacuum ultraviolet photons with solids and gases. Recent work has been concerned with the photon stimulated desorption of atomic and molecular ions from surfaces, with the effect of electric fields on molecular photoabsorption and with the study of molecular photoionization by angle resolved photoelectron spectroscopy. These research programs yield new information about molecular bonding at surfaces, molecular dynamics near ionization thresholds, and the coupling of the electronic and nuclear motion near resonances in molecules. In addition to these programs in basic research SURF-II is used for the calibration of transfer standard detectors over a photon energy range 20 to 250 eV. Calibration of monochromator systems is achieved over the photon energy range 5 to 250 eV by using the now calculable spectral intensity radiated by the electrons, which are confined in a nearly circular orbit. (ERA citation 08:032321)

*601,576*
**DE84004071** PC **A02**/MF **A01**
National Bureau of Standards, Washington, DC.
**Description of the DLC-99/HUGO Package of Photon Interaction Data in ENDF/B-V Format.**
R. W. Roussin, J. R. Knight, J. H. Hubbell, and R. J. Howerton. Dec 83, 23p ORNL/RSIC-46, ENDF-335
Contract W-7405-ENG-26

Keywords: *Photon Transport, *Photons, Beryllium, Coherent Scattering, Computer Codes, Cross Sections, Elements, Form Factors, Hydrogen, Incoherent Scattering, Iron, KeV Range, Lead, Libraries, MeV Range 01-10, MeV Range 10-100, Pair Production, Photoelectric Effect, Uranium, ERDA/654001.

A new photon interaction data library, DLC,-99/HUGO, is described. The library was prepared by incorporating newly evaluated data from the National Bureau of Standards with that from an existing data library, DLC-7F/HPICE, which is the ENDF/B-IV photon interaction data. It contains pair and triplet cross sections, photoelectric cross sections, and atomic form factors and the corresponding coherent scattering cross sections. Evaluated data in INDF/B-V format are provided for elements Z=1 to 100. The data package, available from the Radiation Shielding Information Center

(RSIC) at Oak Ridge National Laboratory, will be submitted to CSEWG for consideration as the ENDF/B-V Photon Interaction Library. Two computer codes, EDPHOT for selectively printing the data and COMP23 for comparing two photon interaction libraries, are also provided. (ERA citation 09:009035)

*601,577*
**DE85013104** PC **A05**/MF **A01**
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Electron Impact Ionization of Multicharged Ions at ORNL: 1980-1984.**
D. C. Gregory, D. H. Crandall, R. A. Phaneuf, A. M. Howald, and G. H. Dunn. May 85, 97p ORNL/TM-9501
Contract AC05-84OR21400

Keywords: *Electron-Ion Collisions, Cross Sections, Data Compilation, Electron Temperature, Experimental Data, Ionization, Ions, ERDA/640304, ERDA/700104.

Experimental electron-impact ionization cross sections for thirty-seven target ions are presented, summarizing measurements made at ORNL during the period from 1980 through early 1984. Target ions range in atomic number from Z = 5 (boron) to Z = 73 (tantalum), with charge states ranging from +2 through +6 and energies ranging from below the ionization threshold to 1500 eV in most cases. All data are presented in both tables and graphs. Maxwellian ionization rate coefficients are tabulated over the equivalent temperature range 10 to 3000 eV, and fitting parameters are given to allow the calculation of rates at intermediate electron temperatures or for inclusion in computer programs for plasma modeling. (ERA citation 10:032502)

*601,578*
**DE86002846** PC **A02**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Source and Instrumentation Div.
**Performance of the 100 keV Chopper/Buncher System of the NBS-Los Alamos RTM Injector.**
M. A. Wilson, R. I. Cutler, D. L. Mohr, S. Penner, and L. M. Young. 1985, 4p DOE/ER/10527-T2
Contracts AT01-79ER10527, W-7405-ENG-36
Pub. in IEEE Transactions on Nuclear Science NS-32, n5 p3089-3091 1985.

Keywords: *Microtrons, Beam Bunchers, Beam Injection, Performance, ERDA/430302.

The purpose of the chopper/buncher system for the RTM injector is to chop a 100 keV 5 mA dc electron beam into 60 exp 0 -long pulses at 2380 MHz and then bunch these beam pulses to 10 exp 0 at insertion into the 5 MeV injector linac. These beam manipulations must contribute a minimum increase in the phase space of the beam such that, at the entrance to the injector linac, the transverse emittance is less than 5 pi mm-mrad. Phase-shift measurements on the chopped beam indicate that the bunching fields are sufficient to achieve the required longitudinal compression. Beam envelope measurements, using wire scanners on the chopped and bunched beam, show that the emittance remains within design goals. (ERA citation 11:006078)

*601,579*
**DE86002849** PC **A02**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Source and Instrumentation Div.
**NBS/LANL Racetrack Microtron Control System.**
R. L. Ayres, N. R. Yoder, E. R. Martin, R. E. Trout, and B. L. Wilson. 1985, 4p DOE/ER/10527-T3
Contracts AT01-79ER10527, W-7405-ENG-36
Also Pub. in IEEE Transactions on Nuclear Science NS-32, n5 p2086-2088 1985.

Keywords: *Microtrons, Computerized Control Systems, ERDA/430300.

The distributed intelligence control system for the NBS/LANL racetrack microtron (RTM) is now nearing completion with all major subsystems implemented and tested, thus providing some operating experience with most of the control system innovations. These include a triple hierarchy of microprocessor-based control elements, consisting of a primary control station and multiple secondary and tertiary control stations; light-link coupling to a tertiary station which operates at a 100 kV potential; a common database shared by separate microprocessors for handling hardware control and operator interactions; and joy stick control of the entire system. A unique secondary station interpreter program was used to great advantage for testing and checkout of various control and monitoring subsystems. The hardware design of the control system is based on Multibus I crates containing commercial Multibus I boards and a few custom designed boards. The primary-secondary data link is a high speed, bidirectional, full-duplex, 8-bit, "byte" parallel link designed for this application. This link permits very fast updating of the monitored data (>5 per second) and timely response to operator control inputs at the primary station. (ERA citation 11:006079)

*601,580*
**PB86-160108** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Photonuclear Reaction Cross Sections for 12C, 14N and 16O.**
Final rept.,
E. G. Fuller. Oct 85, 47p
Pub. in Physics Reports: A Review Section of Physics Letters 127, n3 p185-231 Oct 85.

Keywords: *Carbon 12, *Photonuclear reactions, Nuclear cross sections, Reprints, *Nitrogen 14, *Oxygen 16, Giant resonance.

The results of an evaluation of the available photonuclear-reaction data for (12)C, (14)N and (16)O are presented. While some reaction-yield data are given for energies up to 50 MeV, the primary emphasis is on the excitation-energy range extending from the proton separation energies up to 30 MeV. In addition to photodisintegration measurements, cross-section data derived from inverse particle-capture and electrodisintegration experiments are considered. Data are presented in graphical as well as tabular form. Included in the tables are: energy-weighted moments of the cross sections, bremsstrahlung induced reaction-yield data, radioactive-decay properties of reaction products, and reaction separation energies.

*601,581*
**PB86-160512** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Photon Cross Sections 1 keV to 100 GeV: Current NBS (National Bureau of Standards) Compilation.**
Final rept.,
J. H. Hubbell. 1985, 2p
Pub. in Transactions of the American Nuclear Society 50, p153-154 Nov 85.

Keywords: *Photon cross sections, *Gamma rays, *X-rays, Attenuation, Reprints, KeV range, MeV range, GeV range 01-10, GeV range 10-100.

The current NBS compilation of photon cross section and attenuation coefficient data, developed as part of a continuing project of the NBS Photon and Charged Particle Data Center, is described. Although some mention is made of a new NBS data evaluation project with E. B. Saloman in the soft x-ray region 0.1 keV, the current compilation now being prepared for distribution is for photon energies 1 keV to 100 GeV, including all elements Z = 1 to 100. Associated software by M. J. Berger and S. M. Seltzer, for generating data for arbitrary mixtures of elements, and for arbitrary energies, is also described. Looking to the future, an International Union of Crystallography project, aimed at stimulating new x-ray attenuation coefficient measurements to resolve serious discrepancies in existing 1- to 50-keV data, is mentioned.

*601,582*
**PB86-160520** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
**Experimental Consequences of a Heavy Neutral Fermion.**
Final rept.,
P. M. Fishbane, K. Gaemers, S. Meshkov, and R. E. Norton. 1 Sep 85, 12p
Pub. in Physical Review D 32, n5 p1186-1197, 1 Sep 85.

Keywords: Fermions, Muons, Reprints, *Particle decay, W particle, Z particle, Gauge theory, Electroweak interactions.

The authors study the consequences of adding to the standard model a left-right-symmetric, neutral singlet with a large delta=0 mass. The particle mixes with the standard neutrinos by virtue of the coupling to the conventional Higgs doublet. The authors investigate the effects of both Dirac and Majorana mass mixing on the rare low-energy process mu -> e(gamma) and on the decay of the W and Z. Significant and interesting effects on these latter decays can occur without violating the existing limit on the mu -> e(gamma) decay rate.

*601,583*
**PB86-160538** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Interaction of Quasi-Closed Channels with Open-Channel Continua.**
Final rept.,
P. P. Delsanto, L. C. Biedenharn, and M. Danos. 1985, 4p
Pub. in Lettere al Nuovo Cimento della Societa Italiana di Fisica 42, n2 p59-62 Jan 85.

Keywords: *Nuclear models, *Helium 4, Photonuclear reactions, Reprints.

The Barrett-Delsanto natural boundary-condition treatment of the one-particle continuum is extended to include the interaction with other continua of quasi-closed channels. As an example, the formalism is applied to the study of the quasi-deuteron model of (4)He.

*601,584*
**PB86-160710** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Composite Electron.**
Final rept.,
E. Marx. 1985, 16p
Pub. in International Jnl. of Theoretical Physics 24, n7 p685-700 1985.

Keywords: *Elementary particle theories, *Electrons, *Beta decay, Weak interactions, Electromagnetic interactions, Muons, Pions, Reprints, Intermediate vector bosons, Bound state.

In the paper, the electron is considered a bound state of a neutrino and a negative pion. A model Lagrangian density that combines weak and electromagnetic interactions give rise to equations of motion that define such a state. In the model, the muon is a bound state of an antineutrino and a negative pion, which explains why it cannot decay into an electron and a photon. The decay of unstable particles is reduced to pair creation plus particle recombination. The neutral pion is described by an interference between the charged-pion states. Several variations of the model are also presented.

*601,585*
**PB86-161049** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Glueballs.**
Final rept.,
P. M. Fishbane, and S. Meshkov. 1984, 27p
Grant NSF-PHY81-00257
Sponsored by National Science Foundation, Washington, DC.
Pub. in Comments on Nuclear and Particle Physics 13, n6 p325-351 1984.

Keywords: Reviews, Reprints, *Glueballs.

The current status of various glueball properties such as level ordering, mass, production, and decay is reviewed.

*601,586*
**PB86-163425** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Nuclear Matter under Extreme Conditions.**
Final rept.,
J. Rafelski, and M. Danos. 1985, 94p
Pub. in Proceedings of Summer School, University of Cape Town (South Africa), January 16-27, 1984, Lecture Notes in Physics, p63-156 1985.

Keywords: *High energy particles, Quarks, *Nuclear plasma, Nuclear matter, Gluons.

The report gives an overview of some aspects of hadronic physics relevant for the conception of a research facility devoted to the study of high energy nuclear collisions. Several concepts to be studied in nuclear collisions are selected, with emphasis placed on the properties and nature of the quark-gluon plasma, the formation of the plasma state in the central region and its anticipated lifetime, and the observability,

through strangeness content, of the new form of nuclear matter.

*601,587*
**PB86-163433** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
**Pion Radiation by Hot Quark-Gluon Plasma.**
Final rept.,
J. Rafelski, and M. Danos. 1983, 4p
Pub. in Proceedings of High Energy Ion Study (6th) and Workshop on Anomalons (2nd), Berkeley, CA., June 28-July 1, 1983, p515-518 Dec 83.

Keywords: Quarks, Strong interactions, Antiparticles, Pions, *Nuclear plasma, Quantum chromodynamics, Gluons.

The authors consider an approximately spherical region of the perturbative QCD vacuum, filled with quarks, antiquarks, and gluons. The particle densities are assumed to be reasonably well described by local thermal and chemical equilibrium distributions. The basis for these assumptions is the point that the mean free path of a color-charged particle in the plasma is of the order of 1/3 - 1/2 fm. Outside the perturbation region, colored particles cannot exist and hence any matter found there is in the form of colorless hadrons. Even though indirect evidence supports the picture of the true and perturbative QCD states, they must remember that no direct evidence is available as of now. They regard the observation of the quark-gluon plasma state as the most direct confirmation of the ideas about the nature of strong interactions and quark confinement.

*601,588*
**PB86-163508** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Development of Monoenergetic Electron Beam Sources for Radiation-Instrument Calibration.**
Final rept.,
C. G. Soares, C. E. Dick, J. S. Pruitt, and J. H. Sparrow. 1985, 5p
Sponsored by Nuclear Regulatory Commission, Washington, DC. Office of Nuclear Regulatory Research.
Pub. in Nuclear Instruments and Methods in Physics Research B10/11, p937-941 1985.

Keywords: *Electron beams, *Dosimetry, *Calibrating, Sources, Reprints, *Beta dosimetry, Electron dosimetry.

Accelerator-produced electron beams are being studied for use in obtaining the response of beta-particle dosimetry instrumentation as a function of electron energy. The NBS 4 MV Van de Graaff and 500 kV cascaded rectifier accelerators are being used to generate electron beams from 200 keV to 2.5 MeV. A device capable of scanning the electron beam in two dimensions over an area large enough to cover radiation-survey instruments uniformly is attached to the beam-handling system of each accelerator. The scanned beam exits from vacuum through a 16 sq cm window consisting of either 25 micrometer Kapton (for energies below 500 keV) or 100 micrometer aluminum. The electron beams produced have been characterized in terms of (1) spatial distribution, (2) energy spectrum, and (3) absorbed dose to plastic. Spatial distributions were determined using film, while spectra were measured using a 5 mm-deep Si surface barrier detector. An extrapolation chamber is being used for beam standardization in terms of absorbed dose to plastic.

*601,589*
**PB86-163516** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Bremsstrahlung Spectra from Electron Interactions with Screened Atomic Nuclei and Orbital Electrons.**
Final rept.,
S. M. Seltzer, and M. J. Berger. 1985, 40p
Sponsored by Department of Energy, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in Nuclear Instruments and Methods in Physics Research B12, p95-134 1985.

Keywords: *Photon cross sections, *Bremsstrahlung, Electron scattering, Reprints, Electron-electron collisions, Electron-atom collisions, KeV range, MeV range, GeV range 01-10.

Through the synthesis of various theoretical results, a comprehensive set of bremsstrahlung cross sections (differential in the energy of the emitted photons) has been prepared. The set includes results for electrons with energies from 1 keV to 10 GeV incident on neutral atoms with atomic numbers Z=1 to 100. The paper also contains numerous comparisons between calculated and measured bremsstrahlung spectra, which indicate generally good agreement.

*601,590*
**PB86-175841** PC **A08**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Investigation of Fundamental Interactions with Cold Neutrons: Proceedings of a Workshop.**
Final rept.,
G. L. Greene. Feb 86, 167p NBS/SP-711
Also available from Supt. of Docs as SN003-003-02718-9. Library of Congress catalog card no. 86-600501. Sponsored by Department of Energy, Washington, DC.

Keywords: *Meetings, *Neutrons, *Cold neutrons, National Cold Neutron Facility, Research reactors, Lifetime.

The National Bureau of Standards is establishing a National Cold Neutron Facility at its 20 MW reactor located in Gaithersburg, Maryland. In order to provide guidance in the development of research plans for the Facility, the Department of Energy and NBS sponsored, on November 14-15, 1985, a workshop on the Investigation of Fundamental Interactions with Cold Neutrons. The 25 papers presented at the workshop are printed in the proceedings.

*601,591*
**PB86-185857** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
**Mass Independence of the Electromagnetic Nuclear Response in the Delta Region.**
Final rept.,
J. Ahrens, and J. S. O'Connell. 1985, 11p
Pub. in Comments on Nuclear and Particle Physics 14, n5 p245-255 1985.

Keywords: *Nuclei(Nuclear physics), Electron scattering, Inelastic scattering, Scattering cross sections, Photons, Absorption, Measurement, Reprints, MeV range 100-1000, Response functions.

Recent measurements of the photon absorption and inelastic electron scattering cross sections on nuclei in the excitation region 140-450 MeV show a response that differs from that of a free nucleon but is quite similar (per nucleon) for complex nuclei.

*601,592*
**PB86-186053** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Electrometer Designs for Use in an Unbound-Quark Search.**
Final rept.,
E. R. Williams, and G. T. Gillies. 1983, 5p
Pub. in Lettere al Nuovo Cimento della Societa Italiana di Fisica 37, n15 p520-524 1983.

Keywords: *Electrometers, *Quarks, Searching, Reprints.

An instrument capable of modulating a small capacitance is described. It is to be used as an electrometer in a search for stable fractionally charged particles in test masses of several grams each, the largest yet studied. The new approach uses Gauss's law to sense charge directly and does not require the measurement of small forces as has been the case in most previous quark searches. Preliminary results from an unoptimized experiment are encouraging, showing sensitivities of a few 100 e/(square root of Hz) at atmospheric pressures and without any special precautions.

*601,593*
**PB86-189206** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Absolute Detection Efficiencies of Microchannel Plates for 0.1-2.3 keV Electrons and 2.1-4.4 keV Mg(+) Ions.**
Final rept.,
A. Mueller, N. Djuric, G. H. Dunn, and D. S. Belic. 1986, 5p
Contract DOE-EA-01-A-6010
Sponsored by Department of Energy, Washington, DC.
Pub. in Review of Scientific Instruments 57, n3 p349-353 Mar 86.

Keywords: Electrons, Efficiency, Reprints, *Microchannel electron multipliers, KeV range 01-10, Magnesium ions.

The absolute detection efficiencies of detectors consisting of two microchannel plates (MCP) in a chevron arrangement, were experimentally determined for 0.1-2.3-keV electrons and 2.1-4.4-keV Mg(1+) ions. Both detectors tested included a grid with 92.5% transmission in front of the first MCP. For the measurements, the observed detector count rates were compared to the corresponding particle currents collected in a Faraday cup and measured with a vibrating reed electrometer. The electron detection efficiency of the MCP detector, including the grid, decreases from 0.82 at 0.1 keV to 0.65 at 2.3 keV for electrons incident normal to the surface. The Mg(1+) ion detection efficiency for the same arrangement, but with 43 degree incidence angle, increases from 0.49 at 2.1 keV to 0.81 at 4.4 keV.

*601,594*
**PB86-190659** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Laser Cooling of Atomic Beams.**
Final rept.,
W. D. Phillips. 1984, 1p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Physics Today 37, n1 p26 1984.

Keywords: *Atomic beams, Motion, Reprints, *Laser cooling.

Atomic motion often limits the precision and accuracy with which measurements can be made. Recent experiments at NBS have produced laser - cooled atomic beams where the motion is greatly reduced and is well defined.

*601,595*
**PB86-191905** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**NBS (National Bureau of Standards) Ambient Magnetic Field Meter for Measurement and Analysis of Low-Level Power Frequency Magnetic Fields in Air,**
P. M. Fulcomer. Dec 85, 59p NBSIR-86/3330
Sponsored by Department of Energy, Washington, DC.

Keywords: *Magnetic measurement, *Magnetic fields, Calibrating, Field strength, Magnetometers, Magnetic field meters.

The report describes a portable, battery-powered magnetic fieldmeter which has been developed to provide improved accuracy in the measurement and analysis of low-level and ambient power-frequency magnetic fields. Accurate measurement of such fields is becoming increasingly important as public concern grows over the possibility that exposure to such fields may produce effects on human health. Included in the report are a description of the instrumentation, a circuit analysis, a discussion of the calibration procedures together with an uncertainty analysis, and some sample measurement results. The instrumentation enables measurement of power-frequency magnetic field in air with an overall uncertainty of less than one percent over a range from 50 nanotesla (500 microgauss) to 200 microtesla (2 gauss) and an overall uncertainty of less than two percent down to 2 nanotesla (20 microgauss). It also enables the percentage of each harmonic present in the field to be determined to an uncertainty of less than three percent.

*601,596*
**PB86-191947** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Bibliography of the NBS (National Bureau of Standards) Electromagnetic Fields Division Publications,**
K. A. Gibson, J. M. Page, and C. K. S. Miller. Feb 86, 80p NBSIR-85/3040
Supersedes PB81-143158.

Keywords: *Bibliographies, *Electromagnetic fields, Antennas, Dielectrics, Electromagnetic interference, Microwaves, Metrology, Electromagnetic noise, Remote sensing, Waveforms, Time domain.

The bibliography lists the publications of the personnel of the National Bureau of Standards Electromagnetic Fields Division in the period from January 1970 through September 1985 with selected earlier publications from the Division's predecessor organizations.

*601,597*
**PB86-192440** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
**Electron Production in Proton Collisions: Total Cross Sections.**
Final rept.,
M. E. Rudd, Y. K. Kim, D. H. Madison, and J. W. Gallagher. 1985, 30p
Grants NSF-PHY80-25599, NSF-PHY83-10644
Sponsored by National Science Foundation, Washington, DC., and Department of Energy, Washington, DC.
Pub. in Reviews of Modern Physics 57, n4 p965-994 Oct 85.

Keywords: Proton irradiation, Atoms, Molecules, Electrons, Production, Reprints, *Ionization cross sections.

Existing data on the ionization of neutral atoms and molecules by proton impact are reviewed, and electron production cross-section data are collected. The three major experimental methods are discussed and possible sources of error identified. Some theoretical cross sections are discussed, and well-established methods of relating them to measured cross sections are reviewed. A mathematical equation is fitted to the weighted experimental data for each target, and these fits are adjusted to be consistent with appropriate theoretical calculations and with electron impact and photoionization data. Recommended values of total cross sections for proton-impact ionization are given.

*601,598*
**PB86-192770** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Water Vapor-Enhanced Electron-Avalanche Growth in SF6 for Nonuniform Fields.**
Final rept.,
R. J. Van Brunt. 1986, 10p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in Jnl. of Applied Physics 59, n7 p2314-2323, 1 Apr 86.

Keywords: *Sulfur hexafluoride, *Gas ionization, Water vapor, Reprints, *Electron avalanche.

When water vapor content is increased from 10 to 100 ppm in SF6 at pressures from 200 to 300 kPa, a dramatic enhancement occurs in the mean size of electron avalanches formed near a positive-point electrode. Although the effect can be attributed to a change in gas composition, it is not due to a change in the ionization rate for the gas. It is proposed that the avalanche enhancement is due primarily to an increase in the probability for initiating electron release from minor negative ions associated with water vapor that collisionally detach more readily at a given field strength than the predominant negative ions associated with SF6.

*601,599*
**PB86-193224** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**Collimation of X-rays with Cylindrically Bent, Asymmetrically Cut Crystals.**
Final rept.,
R. Spal. 1984, 3p
Pub. in Nuclear Instruments and Methods in Physics Research Section A-Accelerators Spectro 222, n1-2 p193-195 1984.

Keywords: *X rays, *Collimators, Diffraction, Crystals, Reprints.

Sagittal and meridional collimation of x-rays from a monochromatic point source, using cylindrically bent, asymmetrically cut crystals, is studied. The optimum bending radius and the width of the angular acceptance window are derived analytically, while the degree of collimation is computer numerically.

*601,600*
**PB86-193307** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Gamma-Ray Energies from the Reaction (35)Cl(n,gamma).**
Final rept.,
E. G. Kessler, G. L. Greene, R. D. Deslattes, and H. G. Boerner. 1985, 5p
Pub. in Physical Review C 32, n2 p374-378 Aug 85.

Keywords: Neutron reactions, Gamma rays, Reprints, *Chlorine 35, *Gamma spectroscopy.

A two-axis flat-crystal spectrometer has been used to measure accurately gamma-ray energies up to 2 MeV from the reaction (35)Cl(n, gamma). This represents a fourfold extension of the range of direct optically based gamma-ray energies. The crystals and spectrometer have performed in a manner which demonstrates that sub-ppm measurements are possible at energies approx = or >2 MeV. The reported transition energies (in eV) are given. The sum rule is satisfied by three of the lines within an uncertainty of about 1 ppm.

*601,601*
**PB86-193562** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Energy Loss Straggling of Protons in Water Vapour.**
Final rept.,
M. J. Berger. 1985, 4p
Sponsored by Department of Energy, Washington, DC. Office of Health and Environmental Research, and Office of Naval Research, Arlington, VA.
Pub. in Radiation Protection Dosimetry 13, n1-4 p87-90 1985.

Keywords: *Protons, Water, Reprints, Energy losses, MeV range 01-10, MeV range 10-100.

The paper describes a calculation of energy loss and energy deposition distributions in a 1 micrometer diameter spherical site in a water medium irradiated by 20 MeV or 2 MeV protons. The calculation is designed to indicate the effects of proton energy loss straggling and of energy transport by secondary electrons.

*601,602*
**PB86-193596** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
**Quarks in the Nuclear Ground State.**
Final rept.,
M. Danos, and A. Johnson. 1986, 5p
Pub. in Jnl. of Physics G: Nuclear Physics 12, pL13-L17 1986.

Keywords: *Nuclear structure, *Quarks, Reprints, Bag model, Structure functions.

The authors synthesise the recent deep-inelastic electron scattering data of Arnold et al in terms of a two-component nuclear wavefunction based on the MIT bag model. The quarks in one component are confined to the nucleons while in the other they are free to move over the nuclear volume. An admixture proportional to (A to the 1/3 power) which reaches about 9% for gold reproduces the experimental data well.

*601,603*
**PB86-193901** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
**Direct Determination of the Stored Electron-Beam Current at the NBS (National Bureau of Standards) Electron Storage Ring, SURF-11.**
Final rept.,
A. R. Schaefer, L. R. Hughey, and J. B. Fowler. 1984, 6p
Pub. in Metrologia 19, n4 p131-136 1984.

Keywords: Electron beams, Measurement, Reprints, *Synchrotron Ultraviolet Radiation Facility, *Storage rings.

A method of determining the absolute beam current in the NBS electron storage ring SURF-II by electron counting is described. Recent improvements and the present implementation of the technique are discussed, along with the results of an intercomparison with the NBS spectral irradiance scale.

*601,604*
**PB86-195799** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
**L sup 2 Discretization and Complex Coordinates in the Calculation of Bound-Free Amplitudes in the Presence of Long-Range Forces.**
Final rept.,
B. R. Johnson, and W. P. Reinhardt. Oct 83, 15p
Pub. in Physical Review A 28, n4 p1930-1944 Oct 83.

Keywords: *Potential scattering, Wave functions, Reprints, Discretization(Mathematics), Photoabsorption.

The formalism of Moller wave operators is shown to provide a stable basis for computation of bound-free transition amplitudes for both short and long range potentials without the direct calculation of scattering wave functions. The method, which relies on the techniques of expansion in finite (L sup 2) bases and rotation of the coordinates into the complex plane, is applied to both an exponential potential and one that behaves asymptotically as -1/(r sup 4). It is demonstrated that one obtains not only accurate magnitudes of the matrix elements, but accurate phases (i.e., the scattering phase shift) as well. Some relevant theoretical results with regard to the application of wave operators are also presented. Although couched in terms of potential scattering, the procedures are readily extendible to multichannel problems.

*601,605*
**PB86-196029** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Stereo Presentation of Monte Carlo Electron Trajectory Simulations.**
Final rept.,
D. S. Bright, R. L. Myklebust, and D. Newbury. 1984, 8p
Pub. in Jnl. of Microscopy 136, pt1 p113-120 Oct 84.

Keywords: *Particle trajectories, *Electron beams, *Stereoscopy, Monte Carlo method, Simulation, Reprints, Three dimensional.

Electron trajectory data from Monte Carlo simulation techniques is three dimensional in nature, and thus is best represented by methods that most preserve the spatial information. Stereo plotting is a method that gives the three dimensional illusion effectively while not requiring any special equipment beyond what is required to make standard two dimensional plots. Stereo plots of electron trajectories are presented that illustrate the advantages of the spatial illusion in the context of examining in detail some of the interactions of the electron beam with planar bulk metallic samples.

*601,606*
**PB86-197381** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
**Evaluation of X-ray Loss Due to Electron Backscatter.**
Final rept.,
R. L. Myklebust. 1984, 2p
Pub. in Jnl. de Physique Colloque, nC2 p41-42 1984.

Keywords: *X rays, *Electron scattering, Back scattering, Monte Carlo method, Elastic scattering, Ionization, Attenuation, Microanalysis, Reprints, Electron microprobe analysis.

The loss of x-ray intensity due to backscattered electrons has been re-evaluated with the aid of a Monte Carlo simulation for electron scattering in solids. Initial electron energies in the range 4-50 KeV were considered and the results are presented as the ratio, R, of x-rays generated within the solid to the total x-rays that would have been generated had none of the electrons backscattered. Polynomial fits are presented and the results compared to previous work.

*601,607*
**PB86-199908** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Laser Cooling of Free Neutral Atoms in an Atomic Beam.**
Final rept.,
W. D. Phillips, J. V. Prodan, and H. J. Metcalf. 1983, 6p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Proceedings of International Conference (6th), Laser Spectroscopy 6, Interlaken, Switzerland, June 27-July 1, 1983, p162-167.

Keywords: *Atomic beams, Laser beams, Spectroscopy, *Laser cooling, Sodium atoms.

A free atomic beam of neutral sodium atoms has been decelerated using a near-resonant, counter propagating laser beam. Two methods are described which compensate for the changing Doppler shift of the atoms as they decelerated: Rapidly changing the frequency of the laser, and providing a spatially varying magnetic fields so that the resonant frequency of the atoms changes. Deceleration and dramatic compression of the velocity distribution have been observed for both methods.

*601,608*
**PB86-199916** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.
**Laser Cooling of an Atomic Beam.**
Final rept.,
W. D. Phillips, J. V. Prodan, and H. Metcalf. 1983, 1p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Proceedings of Digest of Technical Papers - Conference on Lasers and Electro-Optics, Baltimore, MD., May 17-20, 1983, p34.

Keywords: *Atomic beams, Frequency standards, Laser beams, Spectroscopy, *Laser cooling, Sodium atoms.

A thermal atomic sodium beam is decelerated and cooled by absorbing photons from a counter propagating laser beam. Final velocities as low as 4% of initial thermal velocities and 'temperatures' of 70 mK have been achieved.

*601,609*
**PB86-200383** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Magnetism in Amorphous Metallic Glasses.**
Final rept.,
J. J. Rhyne. 1983, 28p
Pub. in Proceedings of Summer School at the Ettore Majorana Centre Magnetic Phase Transitions, Erice, Italy, July 1-15, 1983, p241-268.

Keywords: *Magnetization, Neutron scattering, Magnetic properties, *Metallic glasses, Amorphous materials.

No abstract available.

*601,610*
**PB86-200730** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**New Determination of the Deutron Binding Energy and the Neutron Mass.**
Final rept.,
G. L. Greene, E. G. Kessler, R. D. Deslattes, and H. G. Borner. 24 Feb 86, 4p
Sponsored by Institut Max von Laue - Paul Langevin, Grenoble (France).
Pub. in Physical Review Letters 56, n8 p819-822, 24 Feb 86.

Keywords: *Deuterons, *Neutrons, Gamma rays, Reprints, *Binding energy, *Rest mass.

A new value for the deuteron binding energy of B(d) = 2.3881768(24) x 10 to the -3 u is reported based on an absolute wavelength determination of the 2.2-MeV n-p capture gamma ray. Derived values of the n-H and n-p mass differences are also given. The authors also derive M(n)= 1.008 664 919(14) u. The authors note that the uncertainties in the neutron-mass data are now dominated by uncertainties arising from mass spectroscopy.

*601,611*
**PB86-200961** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Streamer Initiation in Liquid Hydrocarbons.**
Final rept.,
G. J. FitzPatrick, E. O. Forster, E. F. Kelley, and R. E. Hebner. Oct 85, 6p
Pub. in Proceedings of Annual Report Conference on Electrical Insulation and Dielectric Phenomena, Amherst, NY., October 20-24, 1985, p27-32.

Keywords: *Electric discharges, *Dielectric breakdown, Hydrocarbons, Insulation, Toluene.

Using 93x magnification and a framing rate of 2 x 10 to the 7th power frames/s, the initiation of prebreakdown streamers in toluene, isooctane, and a white oil have been photographed. The initial growth from a nm a negative point electrode was a thin pencil-like structure, having a growth rate of 2-3 x 10,000 cm/s, which subsequently branched into a tree-like structure. Positive streamers were found to develop into a more filamentary structure than negative streamers. Under nominally identical conditions, a positive streamer may grow then disappear, may grow to bridge the gap, or may grow to a certain length then persist.

*601,612*
**PB86-201753** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
**NBS (National Bureau of Standards) Materials Science Beamlines at NSLS.**
Final rept.,
R. Spal, R. C. Dobbyn, H. E. Burdette, G. G. Long, and W. J. Boettinger. 1984, 4p
Pub. in Nuclear Instrumentation and Methods Phys. Res. Sect. A 222, nl-2 p189-192, 15 May 84.

Keywords: *Synchrotron radiation, Monochromators, Topography, Spectroscopy, Reprints, Small angle scattering, CAMAC system.

Synchrotron radiation beamlines for topography, spectroscopy, and small angle scattering, at energies from 5 to 20 keV, are described.

*601,613*
**PB86-201787** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
**Scattering of Transient Waves by a Dispersive Body.**
Final rept.,
E. Marx. 1983, 4p
Pub. in Proceedings of the International Symposium Digest - Antennas and Propagation (1983), Houston, TX., May 23-26, 1983, p26-29. Sponsored by Antennas and Propagation Society (IEEE), New York.

Keywords: *Electromagnetic scattering, Electromagnetic fields, Wave equations, Transient waves.

A transient electromagnetic field interacts with a conducting body. The permittivity and conductivity of the medium generally depend on frequency, that is, the medium is dispersive. Instead of decomposing the pulse into its Fourier components, the determination of the scattered and transmitted fields can be carried out in the time domain to take advantage of marching-in-time procedures. Maxwell's equations and the derivation of the fields from a single tangential vector field that obeys a singular integral equation are suitably modified. A simple conductor is presented as an example.

*601,614*
**PB86-201951** PC **A05**/MF **A01**
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
**Composite Proton,**
E. Marx. Apr 86, 91p NBSIR-86/3370

Keywords: *Elementary particle theories, *Nuclear models, Strong interactions, Weak interactions, Electromagnetic interactions, Leptons, Relativity, Strange particles, Hadrons, Quantum mechanics, Bound state, Beauty model, Charm particles, Composite models, Nuclear resonance.

A model is proposed in which the proton and other baryons are particles composed of only two basic particles: an archaeobaryon (archyon) and one or more pions. Mesons are composed of pions alone. A third basic particle is the neutrino, which is a component of all leptons. The interactions between the three corresponding fields and the electromagnetic field are derived from a Lagrangian density that has only two masses and three coupling constants. The interactions are expressed in terms of conserved currents, one for each particle. All particle reactions are reduced to four processes: particle scattering, antiparticle scattering, pair creation, and pair annihilation. The last two correspond to the reflection of the wave function in the time direction. There is no longer a need for a separate theory of unstable particles. The pion is the only electrically charged particle, which accounts for the equality of the magnitude of all charges of elementary particles. Strong and weak interactions of hadrons are different manifestations of a single interaction; the distinction is related to pair creation or annihilation, energy barriers, and the flux of particles and antiparticles.

*601,615*
**PB86-201993** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
**Siegert's Theorem and Nuclear Electrodisintegration.**
Final rept.,
W. R. Dodge, and E. Hayward. Apr 86, 7p
Sponsored by Lewes Physics Center, DE.
Pub. in Physical Review C 33, n4 p1251-1257 Apr 86.

Keywords: Electron scattering, Scattering cross sections, Photons, Reprints, *Siegert theorm, *Electrodisintegration, Form factors, Virtual particles.

The connection between the electron scattering electric dipole coincidence cross section, (e,e'X), and the inclusive electric dipole (e,X) cross section, differential in the angle of the outgoing X particle, is derived. Unlike the (e,e') inclusive cross section which contains contributions from only two of the four terms of the (e,e'X) cross section, the (e,X) cross section contains contributions from all four terms of the (e,e'X) cross section. Data from a previous experiment have been used to obtain the magnitude and sign of the interference term between the transverse and Coulomb reduced matrix elements (form factors) in the limit as q -> omega, from the relationship commonly referred to as Siegert's theorem in the context of inclusive (e,e') scattering.

*601,616*
**PB86-202017** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Shell-Model Interaction Energies in a Relativistic Hamiltonian Formulation (1).**
Final rept.,
T. Kohmura, T. Suzuki, M. Cauvin, M. Danos, and V. Gillet. 1986, 24p
Pub. in Nuclear Physics A 449, p729-749 1986.

Keywords: *Nuclear shell models, *Mesons, Field theory(Physics), Relativity, Hamiltonian functions, Reprints.

The non-covariant Hamiltonian formulation of relativistic field theory is presented and solved as a secular problem in a discrete representation space. The shell-model two-nucleon interaction in the one-boson exchange picture is used to test the method before applying it to many-body systems. The results of the diagonalization treatment are convergent as a function of the discretized meson space and are close to the usual OBEP when considering the exchange of a single type of meson, thus establishing the numerical feasibility of the method. However a significant deviation between the two approaches appears for the sigma meson or for a mixture of several types of mesons with values of the coupling constants in the 'physical' domain. Also, in the limited momentum space of the nucleons in the lowest shell-model state, the cut-off in the nucleon vertex form factors plays an unimportant role.

*601,617*
**PB86-202389** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Quantum-Mechanical Noise and Squeezed-State Technique in an Interferometer.**
Final rept.,
W. T. Ni. 1984, 2p
Pub. in Proceedings of the Congress of the International Commission for Optics (13th), Sapporo, Japan, August 20-24, 1984, Optics in Modern Science and Technology, p48-49.

Keywords: Uncertainty principle, *Gravitational wave detectors, *Quantum noise, Laser interferometers.

Several groups around the world are now developing laser interferometers to detect gravitational waves by measuring small relative position changes of suitably separated masses. The fundamental limitations on the sensitivity of such interferometers come from quantum-mechanical noise while the sensitivity of the present gravitational-wave detectors is mainly limited by intensity fluctuations and therefore by power. In the paper we address the problem of correlations of different sources of quantum-mechanical noise and investigate the use of squeezed-state technique in optimizing the power requirement.

*601,618*
**PB86-208428** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Effect of Pressure on Streamer Initiation In n-Hexane.**
Final rept.,
E. F. Kelley, R. E. Hebner, G. J. FitzPatrick, and E. O. Forster. 1986, 3p
Pub. in Conference Record 1986 IEEE (Institute of Electrical and Electronics Engineers) International Symposium on Electrical Insulation, Washington, DC., June 9-11, 1986, p66-68.

Keywords: *Electric discharges, *Hexanes, *Dielectric breakdown, *Electrical faults, Aliphatic hydrocarbons, High speed photography, Electrical insulation, Pressure effects.

High speed photographs of the breakdown process at pressures in the range 0.1-10 MPa indicate that the structure of the streamer changes with the pressure. The typical structures associated with primary streamers are no longer visible at elevated pressures. Over this range, the average cathode streamer velocity increases from about 0.25 km/s to 2.5 km/s. The anode streamer, however, does not generally exhibit a bushy primary streamer structure and its velocity appears to be less affected by pressure.

*601,619*
**PB86-209327** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**High-Speed Data Systems for Pulsed Power Applications.**
Final rept.,
R. E. Hebner. 1986, 4p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Pulsed Power Conference (5th), Arlington, VA., June 10-12, 1985 p168-171 May 86.

Keywords: *Data aquisition, *Electrooptics, *Magnetooptics, Calibration, Electromagnetic interference, Standards, Errors, Pulsed power.

Data acquisition systems for pulse power applications generally must provide nanosecond resolution, operate in an environment of high levels of electromagnetic interference, and acquire significant amounts of data simultaneously. To meet these demands, electrical systems have been used and optical systems are being introduced. Voluntary standards have been and are being developed which categorize the errors in the electrical measurement systems. The development of optical systems is too immature for similar standardization.

*601,620*
**PB86-209335** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Electro-Optical Measurement Techniques.**
Final rept.,
R. E. Hebner. 1986, 21p
Pub. in Fast Electrical and Optical Measurements 1, p5-25 1986.

Keywords: *Electrooptics, *Measurement, Electric fields, Magnetic fields, Currents, Electric potential, Electric charge, Faraday effect, Kerr electrooptical effect, Birefringence, Reprints.

The paper reviews the use of the Faraday effect, the Pockels effect, and the Kerr effect to measure electric fields, magnetic fields, voltages, currents, and space charge density. Each of the three effects is introduced conceptually, the use of Jones or Mueller matrices to describe the optical system is presented, and some applications of these effects are described.

*601,621*
**PB86-209962** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
**Transformation of Time-Domain Relaxation Data into the Frequency Domain.**
Final rept.,
F. I. Mopsik. 1985, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electrical Insulation EI-20, n6 p957-964 Dec 85.

Keywords: *Dielectrics, Laplace transformation, Errors, Numerical integration, Numerical analysis, Reprints, Frequency domain, Time domain.

A numerical technique is developed for computing the Laplace transform of the time-domain behavior of a dielectric in order to obtain its frequency-domain behavior. The method is based on fitting a cubic spline to the original data and using the spline to define the integration. The error in the computation is investigated for data uniformly spaced on a logarithmic time scale. It is shown that the error is much smaller than with previous methods, is computationally stable, and converges as the fourth power of the sample density. For an error of 0.0001 or less, only 10 points per decade are required for all frequencies that correspond to the time window of the measurement. It is also shown that it is possible to estimate those parts of the integrals that lie outside the measurement window from the data inside the window, so that the errors from the unknown parts are kept small and affect only the extremes of the frequency range.

*601,622*
**PB86-210051** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Fundamental Properties of the Neutron.**
Final rept.,
G. L. Greene. 1986, 5p
Pub. in Physica B 136, p121-125 1986.

Keywords: *Neutrons, Reviews, Reprints.

In addition to providing a probe of great power in condensed matter and nuclear research, the neutron itself is the object of a considerable research effort. The study of the properties of the neutron can shed light on a variety of questions in particle physics, cosmology, astrophysics, and nuclear physics. A summary of the neutron properties is given, along with the methods used for their determination and their theoretical implications.

*601,623*
**PB86-210077** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Electron Beam Bunch Profile Determination Through Cerenkov Radiation.**
Final rept.,
X. K. Maruyama, J. R. Neighbours, and F. R. Buskirk. 1985, 3p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science NS-32, n5 p1994-1996 Oct 85.

Keywords: *Electron beams, *Cerenkov radiation, Air, Reprints, Beam profiles, Relativistic range.

The spatial charge distribution of an electron pulse, along with the beam interaction length, determines the Cerenkov radiation distribution as a function of frequency. An angular distribution of the Cerenkov radiation can, in principle, measure its spatial charge distribution. At a measurement angle of 90 degrees with respect to the beam direction, the form factor is unity which allows a measurement of the total charge contained in the pulse. At other angles, Fourier transforms of the charge distribution may be measured. Possible application to intense relativistic beams in air is discussed.

*601,624*
**PB86-210747** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Space Experiments: Report of Workshop C2.**
Final rept.,
P. L. Bender. 1984, 9p
Pub. in Proceedings of International Conference on General Relativity and Gravitation (10th), Padova (Italy), July 31, 1983, p387-395 1984.

Keywords: *General relativity, *Gravitational waves, Hipparcos satellite, Galileo project, Pulsars, Satellites.

A number of tests of gravitational physics using planned or proposed new space missions were discussed at the Workshop. Among these were the following: the Stanford Gyro Relativity Experiment, which would test the 'gravitomagnetic' effects predicted by general relativity for the first time; new calculations of small relativistic effects for accurately tracked earth satellites; light-bending observations by the HIPPARCOS satellite; planned low-frequency gravitational wave experiments during the Galileo and ISPM missions; and limits on very-low-frequency gravitational waves from pulsar timing measurements.

*601,625*
**PB86-213014** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Source and Instrumentation Div.
**Progress Report on the NBS/Los Alamos RTM (Racetrack Microtron).**
Final rept.,
S. Penner, R. L. Ayres, R. I. Cutler, P. H. Debenham, and E. R. Lindstrom. 1985, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science NS-32 n5 p2669-2671 Oct 85.

Keywords: *Electron accelerators, Reprints, *Racetrack microtrons, *Microtrons.

The NBS-Los Alamos 200 MeV Racetrack Microtron is being built under a program aimed at developing the technology needed for high-current intermediate-energy CW electron accelerators. The authors give an overview of the present status of the project. Recent progress is discussed.

*601,626*
**PB86-213022** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Source and Instrumentation Div.
**End Magnets for the NBS-Los Alamos Racetrack Microtron.**
Final rept.,
P. H. Debenham, E. R. Lindstrom, and D. L. Mohr. 1985, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science NS-32, n5 p3648-3650 Oct 85.

Keywords: *Magnets, Magnetic fields, Reprints, *Microtrons, *Racetrack microtrons.

Two end magnets have been designed and constructed for the 185 MeV NBS-Los Alamos racetrack microtron. The field has been measured in the first magnet and is uniform over a 0.62 sq m area to within + or - 0.0002 at 1 T. The magnet meets all performance specifications. Field measurements are underway on the second magnet. In this paper, design and construction details which play an important role in magnetic performance are described, and the measured fields are compared with calculations.

*601,627*
**PB86-213048** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
**Heat-Capacity Calorimetry by the Method of Mixtures.**
Final rept.,
D. A. Ditmars. 1984, 27p
Pub. in Compendium of Thermophysical Property Measurement Methods: Survey of Measurement Techniques, v1 p527-553 1984.

Keywords: *Calorimeters, *Heat measurement, Enthalpy, Specific heat, Thermodynamics, Reprints.

The field of calorimetry, using the method of mixtures, to measure relative enthalpy and heat capacity is surveyed. The aim is to present for the non-specialist in the technique sufficient material concerning its areas of strength and its limitations to assist him in deciding whether or not the technique is applicable to his measurement problem. Following an introduction giving the basic thermodynamic theory of the calorimetric technique, specific calorimeter types are discussed. For each type, basic operating principles, range of utility, strengths, weaknesses and special problems are covered. A comprehensive bibliography of references to applicable calorimetric instrumentation is presented together with brief commentary on salient features of the references.

*601,628*
**PB86-229705** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Application of the Dual Thin Scintillator Neutron Flux in a (235)U(n,f) Cross-Section Measurement.**
Final rept.,
M. S. Dias, A. D. Carlson, R. G. Johnson, and O. A. Wasson. Jun 85, 4p
Pub. in Proceedings of International Atomic Energy Agency (IAEA) Advisory Group Meeting on Nuclear Standard Reference Data, Geel, Belgium, November 12-16, 1984, p467-470 1985.

Keywords: *Uranium 235, *Fission cross sections, *Neutron cross sections, Neutron flux, MeV range 01-10, Time-of-flight method, Neutron detectors.

The fission cross section for (235)U was measured over the 1 to 6 MeV energy range using the National Bureau of Standards neutron time-of-flight facility at the NBS 100-MeV electron linac. The recently developed dual thin scintillator (DTS) neutron detector was used as the neutron flux monitor. The DTS flux monitor was placed about 200 m from the source. At about 69 m on the same flight path, a well-characterized fission chamber containing about 100 micrograms/sq cm of (235)U was located. The background for both detectors was reduced to negligible levels. Two parameter data (pulse height and time-of-flight) were taken for both detectors with a computer based system. Since the experiment was devised primarily to verify the accuracy of the DTS detector as an absolute neutron flux monitor, only moderate energy resolution was planned (delta E/E = 10%). The cross section uncertainty obtained was about 2%.

*601,629*
**PB86-229713** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Physics Div.
**Neutron Cross-Section Standards Evaluations for ENDF/B-VI.**
Final rept.,
A. D. Carlson, W. P. Poenitz, G. M. Hale, and R. W. Peelle. Jun 85, 8p
Pub. in Proceedings International Atomic Energy Agency (IAEA) Advisory Group Meeting on Nuclear Standard Reference Data, Geel, Belgium, November 12-16, 1984, p77-84 Jun 85.

Keywords: *Neutron cross sections, *Standards, Uranium 235, Hydrogen, Neutron reactions, R matrix, Lithium 6, Boron 10, Gold 197.

As a first step in the development of the new ENDF/B-VI file, the neutron cross section standards are being evaluated. These standards evaluations are following a different process compared with that used for earlier versions of ENDF. The primary effort is concentrated on a simultaneous evaluation using a generalized least squares program, R-matrix evaluations, and a procedure for combining the results of the evaluations. The ENDF/B-VI standards evaluation procedure is outlined, and preliminary simultaneous evaluation and R-matrix results are presented.

*601,630*
**PB86-231479** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Do Heavy Quarkonia Have Stringlike Behavior.**
Final rept.,
P. M. Fishbane, P. Kaus, and S. Meshkov. 1986, 4p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review D: Particles and Fields 33, n3 p852-855, 1 Feb 86.

Keywords: Reprints, *String models, *Quarkonium.

It is shown that heavy q(q bar) systems can be described for r > (R sub c) by the square-root potential K(square root of (r squared - (R sub c) squared)) + (V sub 0) characteristic of strings. (R sub c) approx. = 0.3 fm, a number consistent with Nambu-Goto strings.

*601,631*
**PB86-239399** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Optical and Spectral Characteristics of an Insertion Device Used Both as a Wiggler and an Undulator.**
Final rept.,
S. Brennan, P. L. Cowan, T. Jach, R. LaVilla, and R. C. C. Perera. 1986, 4p
Sponsored by Department of Energy, Washington, DC., and National Institutes of Health, Bethesda, MD.
Pub. in Nuclear Instruments and Methods in Physics Research A246, p37-40 1986.

Keywords: Reprints, *X-ray sources, Wiggler magnet, Undulators.

For experiments using the energy region below 4 keV the LBL/EXXON insertion device on Beam Line VI-2 at the Stanford Synchrotron Radiation Laboratory (SSRL) can be reconfigured to work as a source of undulator radiation. For example, with a K of 0.94 rather than its normal value of 5-8 the fourth harmonic of the undulator coincides with the Ar K absorption edge at 3.2 keV. Because the total power is relatively low, carbon foils protecting the beryllium window can be removed. Thus there is a net gain the flux at the Ar edge over that obtainable in wiggler mode with carbon absorbers in place. In addition, the beam transmitted by the monochromator has a lower harmonic content and improved energy resolution.

*601,632*
**PB86-239407** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**High Energy Resolution X-ray Spectroscopy Synchrotron Radiation Beamline for the Energy Range 800-5000 eV.**
Final rept.,
P. L. Cowan, S. Brennan, R. D. Deslattes, A. Henins, and T. Jach. 1986, 5p
Pub. in Nuclear Instruments and Methods in Physics Research A246, p154-158 1986.

Keywords: *Synchrotron radiation, X ray spectroscopy, Monochromators, Mirrors, Reprints, *X-ray sources, NSLS, eV range 100-1000, KeV range 01-10.

A beamline for X-ray spectroscopy of atomic and molecular gases and condensed matter has been designed and installed at the National Synchrotron Light Source. The beamline is UHV compatible to allow windowless operation for improved flux at low photon energies. A double axis crystal monochromator is employed with a collimating premirror and a focusing postmirror. Pairs of beryl, quartz, or silicon crystals define an energy band width of <0.4 eV at an arbitrary energy above 0.8 keV. The premirror acts as a tuneable low-pass filter to minimize heat loading on the first monochromator crystal. At the present operating parameters of NSLS, a flux of 10 to the 9th power - 10 to the 13th power photons/s of highly monochromatic X-rays can be focused onto a 1mm diameter spot. Initial experimental results are presented.

*601,633*
**PB86-240447** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Comment on 'Reanalysis of the Eotvos Experiment'.**
Final rept.,
P. T. Keyser, T. Niebauer, and J. E. Faller. 1986, 2p
Pub. in Physical Review Letters 56, n22 p2425-2426, 2 Jun 86.

Keywords: Gravitation, Reprints, *Eotvos experiment.

Fischbach et al. (Phys. Rev. Lett. 56, 3 (1986)) present an analysis of the Eotvos, Pekar, and Fekete data from which they suggest the presence of a non-Newtonian coupling to baryon number (i.e., hypercharge). The authors find two flaws: (a) they misinterpret or omit some of the Eotvos et al. data and (b) they reject the work of Janos Renner.

*601,634*
**PB86-240454** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Radiative-Transfer Equations in Broad-Band, Time-Varying Fields.**
Final rept.,
J. Cooper, and P. Zoller. 1984, 7p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Astrophysical Jnl. 277, n2 p813-819 1984.

Keywords: Maxwell's equations, Reprints, *Radiative transfer, Wigner function.

A derivation of the equation of transfer is obtained by starting with Maxwell's equations in the 'slowly varying envelope' form. Particular attention is paid to characterizing the intensity that is 'seen' by the atom (which is found to be related to a Wigner distribution of the electric field). The equation of transfer is found to be valid for 'broadband' slowly varying radiation fields.

*601,635*
**PB86-241908** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Physics Div.
**Absolute Measurements of the (235)U(n,f) Cross-Section for Neutron Energies from 0.3 to 3 MeV.**
Final rept.,
A. D. Carlson, J. W. Behrens, R. G. Johnson, and G. E. Cooper. Jun 85, 5p
Pub. in Proceedings International Atomic Energy Agency (IAEA) Advisory Group Meeting on Nuclear Standard Reference Data, Geel, Belgium, November 12-16, 1984, p162-166 Jun 85.

Keywords: *Uranium 235, *Neutron cross sections, *Fission cross sections, MeV range 01-10, KeV range 100-1000.

Measurements of the (235U) neutron fission cross section have been made at the NBS linac neutron time-of-flight facility. The neutron flux was measured with a Black Neutron Detector located at the 200 m experimental station of the facility. The fission events were detected with a well-characterized (235U) fission ionization chamber located 69 m from the neutron producing target on the same beam line as the Black Detector. The data have been grouped to statistical precisions of about 1%. Total uncertainties are about 2%.

*601,636*
**PB86-241916** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
**Tritium Form-Factors at Low q.**
Final rept.,
D. H. Beck, S. B. Kowalski, M. E. Schulze, W. E. Turchinetz, and J. W. Lightbody. 1984, 6p
Pub. in Physical Review C: Nuclear Physics 30, n5 p1403-1408 1984.

Keywords: *Tritium, Reprints, *Form factors.

The elastic charge and magnetic form factors of (3)H have been measured in the region 0.0477 < q sup 2 < 2.96/fm squared. Throughout this range, the charge form factor is found to be larger than previous measurements whereas the magnetic form factor agrees with the earlier work. The change in the charge form factor increases the discrepancy between the calculated and observed binding energy difference between (3)H and (3)He.

*601,637*
**PB86-241924** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Physics Div.
**Comparison of the Filtered-Neutron Beams at the NBS and PTB Reactors by Calibrating a Spherical Rem Meter.**
Final rept.,
W. G. Alberts, and R. B. Schwartz. 1985, 8p
Pub. in Commission European Communities Report EUR-9762, Radiation Protection 1, p629-636 1985.

Keywords: *Neutron beams, Calibrating, Comparison, Reprints, Remmeters.

Two filtered-neutron beam facilities at the NBS and at the PTB, providing quasi-monoenergetic beams of 2 keV, 24.5 keV and 144 keV, are in use for radiation protection instrument calibration. Measurements are described which were performed to investigate the properties, and compare the calibrations, of these beams at both installations. A 20.8 cm diameter spherical rem counter and an 11 cm diameter sphere served as transfer instruments. The neutron current in the beams was determined with the respective methods in use at either facility. A filter-difference method was used to determine the contribution of high-energy neutron contamination to the count rate of the instruments. The responses of the instruments to the quasi-monoenergetic neutrons at both institutes are compared.

*601,638*
**PB86-247574** PC **A04**/MF **A01**
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Transient Losses in Superconductors.**
Final rept. 1 Oct 82-30 Sep 85,
R. B. Goldfarb. Jun 86, 63p NBSIR-86/3053
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Superconductors, Type 2 superconductors, Hysteresis, Magnetization, Magnetometers, Niobium, Filaments, Titanium, Alternating current.

The report deals with hysteresis losses at 4 K measured by magnetization and complex magnetic susceptibility. The theoretical and experimental relationships between ac susceptibility and magnetization as functions of dc field were examined in terms of the critical-state model as developed by Carr and Clem. A theoretical method of calibrating ac susceptometers for cylindrical specimens, which is based on a mutual-inductance calculation, was developed.

*601,639*
**PB87-102422** PC **A99**/MF **E04**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**X-ray Attenuation Coefficients (Total Cross Sections): Comparison of the Experimental Data Base with the Recommended Values of Henke and the Theoretical Values of Scofield for Energies between 0.1-100 keV,**
E. B. Saloman, and J. H. Hubbell. Jul 86, 715p
NBSIR-86/3431
Sponsored by Department of Energy, Washington, DC., and Department of the Navy, Washington, DC.

Keywords: *X rays, *Absorption cross sections, Tables(Data), Graphs(Charts), Comparison, *Absorption coefficients, Total cross sections, eV range 100-1000, KeV range 1-10, KeV range 10-100, Photon-atom collisions.

A comparison is carried out, in both graphical and tabular form, over the energy range 0.1-100 keV between the National Bureau of Standards' data base of experimental x-ray attenuation coefficients (total absorption cross sections) and cross sections obtained using two sets of photoionization cross section values: the semi-empirical set of recommended values produced by Henke et al which covers the energy range .03-10 keV; and a theoretical set calculated by Scofield which covered the range 1-1500 keV and was extended by Scofield, at our request, to also cover the 0.1-1 keV range. There has been some disagreement over whether Scofield's results should be subject to renormalization from a Hartree-Slater to a Hartree-Slater to a Hartree-Fock atomic model. Therefore in the tables a comparison is made of Scofield's predictions both with and without the renormalization.

*601,640*
**PB87-102901** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Coordinate Time in the Vicinity of the Earth.**
Final rept.,
D. W. Allan, and N. Ashby. 1986, 15p
Pub. in Proceedings of International Astronomical Union Symposium No. 114-Relativity in Celestial Mechanics and Astrometry, Leningrad (USSR), May 28-31, 1985, p299-313 1986.

Keywords: *Atomic clocks, General relativity, Accuracy, Comparison, Time standards, Frequency standards.

Atomic clock accuracies continue to improve rapidly, requiring the inclusion of general relativity for unambiguous time and frequency clock comparisons. Atomic clocks are now placed on space vehicles and there are many new applications of time and frequency metrology. The paper addresses theoretical and practical limitations in the accuracy of atomic clock comparisons arising from relativity, and demonstrates that accuracies of time and frequency comparison can approach a few picoseconds and a few parts in 10 to the 16th power, respectively.

*601,641*
**PB87-104071** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Characterization, Optimum Estimation, and Time Prediction of Precision Clocks.**
Final rept.,
D. W. Allan. 1986, 23p
Pub. in Proceedings of Annual Precise Time and Time Interval Applications (17th) and Planning Meeting, Washington, DC., December 3-5, 1985, p45-67 1986.

Keywords: *Atomic clocks, Standard deviation, Performance, Reviews, Precision, Optimization.

The paper is a partial review of several other papers given in the reference per the guidelines of the title. A few additional calculations are added for completeness of some of the tables, which indicate the uselessness of the standard deviation for a measure of performance of atomic clocks. A proper characterization of both the low-frequency, divergent-power-law processes observed for the random deviations of precision oscillators as well as the environmental sensitivities and systematic characteristics opens the door to: a clear characterization of performance; optimum estimation procedures of systematic parameters; optimum estimation of the influence of environmental parameters; optimum prediction algorithms; and clear specifications which allow system designers and planners to estimate the influence of a given precision oscillator on their system.

*601,642*
**PB87-104469** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
**Nonlinearity in Weak Magnetic Fields Induced by Neutron-Antineutron Oscillations in Neutron Interferometry and Spin Resonance.**
Final rept.,
R. C. Casella. 1984, 4p
Pub. in Physical Review Letters 53, n11 p1033-1036 1984.

Keywords: Magnetic fields, Baryons, Nuclear spin, Reprints, *Neutron oscillation, Grand unified theory, Nuclear resonance, Nonlinearity.

In principle these minute effects are observable if regeneration problems can be overcome, but general statistical arguments render this approach non-competitive with direct observation of the neutron.

*601,643*
**PB87-105177** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Research on Practical Superconductors at National Bureau of Standards.**
Final rept.,
F. R. Fickett. 1985, 7p
Pub. in ATB Metallurgie 25, n4 p265-271 1985.

Keywords: *Superconductors, *Superconducting magnets, Critical field, Copper, Stability, Reprints, Critical current.

The National Bureau of Standards is engaged in a large number of research programs which have as their goals the evaluation of various properties of practical superconductors related to their application in large magnet systems. The NBS work has concentrated on measurement of critical current, critical field, ac losses, and properties of the copper normally used as a stabilizing material. Many parameters must be considered in these investigations. An overview of these research efforts and a selection of recent results are presented. Particular emphasis is given to work performed in cooperation with the International Copper Research Association (INCRA) on properties of oxygen-free copper.

*601,644*
**PB87-106415** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
**Anomalous Vertical Magnetic Field for Electromagnetic Induction in a Laterally Varying Thin Conductive Sheet.**
Final rept.,
D. A. Hill, and J. R. Wait. 1986, 5p
Sponsored by Bureau of Mines, Washington, DC.
Pub. in Radio Science 21, n4 p617-621 Jul-Aug 86.

Keywords: *Electromagnetic induction, Magnetic fields, Surface resistivity, Electromagnetic fields, Reprints.

The authors employ a simple model to show how the natural electromagnetic field on the surface of the earth, which has a strong horizontal magnetic field component, can be converted to a significant vertical magnetic field at the surface. Such a conversion mechanism will be caused by lateral variations of the subsurface conductivity structure. Our idealized model is a thin conducting sheet with a periodic variation of the conductivity-thickness product in one horizontal direction only.

*601,645*
**PB87-106712** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Implementation of CRCPD Accreditation Criteria in State Calibration Laboratories.**
Final rept.
H. T. Heaton. 1985, 18p
Contract DE-AC06-76RLO-1830
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of Workshop on Radiation Survey Instruments and Calibrations, Gaithersburg, MD., July 10-12, 1984, pD.22-D.39 1985.

Keywords: *Laboratories, *Test facilities, *Calibrating, *Ionizing radiation, Quality control, Accreditation.

The paper summarizes the unique aspects of the four state laboratories for calibrating ionizing radiation instruments, with which NBS is presently cooperating. The general requirements of the CRCPD accreditation criteria are reviewed, and the procedures by which the state labs meet the criteria are discussed.

*601,646*
**PB87-110102** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
**Electron Scattering by Neon in Resonance Regions.**
Final rept.,
K. T. Taylor, C. W. Clark, and W. C. Fon. 1985, 15p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, p2967-2981 1985.

Keywords: *Electron scattering, *Neon, Inelastic scattering, Atomic structure, Reprints.

The authors present cross sections for excitation and de-excitation of neon by electron impact at energies up to 20 eV above the ground state, calculated by the R-matrix method. Comparison with available experimental data is satisfactory, and a number of transitions between excited states are examined theoretically for the first time. The effect of resonances on the cross section is seen to be quite large in some instances. In addition, calculated values of the oscillator strength and transition probabilities for the 3s-3p transition array of neon are given, and are compared with other recent theoretical and experimental values.

*601,647*
**PB87-110201** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Future Atomic Frequency and Time Standards.**
Final rept.,
D. J. Wineland. 1981, 12p
Pub. in Seminar on Frequency Standards Measurement and Usage, Basancon (France), March 23-25, 1981, p1-12.

Keywords: *Frequency standards, *Time standards, Atomic beams, Atomic clocks, Cesium frequency standards, Rubidium frequency standards, *Ion storage.

Research towards making improved primary microwave frequency and time standards is reviewed. Two areas are highlighted (1) Advances in atomic beam research, and (2) Prospects for stored ion frequency standards.

*601,648*
**PB87-110219** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Research on Field Usable Cs and Rb Frequency Standards.**
Final rept.,
D. J. Wineland. 1981, 17p
Pub. in Seminar on Frequency Standards Measurement and Usage, Besancon (France), March 23-25, 1981, p1-17.

Keywords: *Cesium frequency standards, *Rubidium frequency standards, *Frequency standards, Atomic clocks, Time standards, Reviews, Ion storage.

Current research towards improving the 'physics packages' in field-usable Rb and Cs clocks is reviewed. The paper is intended to update other similar reviews.

*601,649*
**PB87-110227** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

**Optical Pumping of Stored Atomic Ions.**
Final rept.
D. J. Wineland, W. M. Itano, J. C. Bergquist, J. J. Bollinger, and J. D. Prestage. 1985, 12p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Ann. Phys. Fr. 10, p737-748 Dec 85.

Keywords: *Optical pumping, Atomic spectroscopy, Reprints, *Ion storage, Laser cooling, Laser spectroscopy, Ion traps.

Optical pumping experiments on atomic ions which are stored in electromagnetic <<traps>> are discussed. Weak relaxation and extremely small energy shifts of the stored ions lead to very high resolution and accuracy in optical pumping-double resonance experiments. In the same spirit of Kastler's proposal for <<lumino refrigeration>> (1950), the kinetic energy levels of stored ions can be optically pumped. This technique, which has been called laser cooling, significantly reduces Doppler frequency shifts in the spectra.

*601,650*
**PB87-110235** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Frequency Standards Based on Stored Ions.**
Final rept.,
D. J. Wineland. 1986, 4p
Sponsored by Office of Naval Research, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Proceedings of the Institute of Electrical and Electronics Engineers 74, n1 p147-150 Jan 86.

Keywords: *Frequency standards, Atomic spectroscopy, Atomic clocks, Reprints, *Ion storage, Laser cooling, Laser spectroscopy.

The state of development of frequency standards based on stored ions is reviewed. Several preliminary demonstrations of the concept have already shown a level of performance approaching that of today's cesium-beam standards (accuracy of one part in 10 to the 13th power). The potential for accurately measuring or reducing all known systematic effects suggests that frequency standards based on stored ions with inaccuracies of one part in 10 to the 15th power are obtainable and eventually they could be orders of magnitude better than this. This performance is a result of extremely high-Q resonances (e.g., millihertz linewidths at microwave frequencies) and a very small second-order Doppler shift which follows with the addition of techniques for ion cooling.

*601,651*
**PB87-111068** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Some Remarks on the Interaction between Precision Physical Measurement and Fundamental Physical Theories.**
Final rept.,
J. L. Hall. 1983, 15p
Grants N0001477-C-0656, NSF-PHY79-04928
Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in Quantum Optics, Experimental Gravity, and Measurement Theory, p347-361 1983.

Keywords: *Special relativity, *Lorentz transformations, Atomic beams, Precision, Tests, Laser interferometry.

Physicists have been unreasonably successful in framing physical 'laws' by idealization of rather crude experimental results. The author states 'unreasonably' successful because such fundamental physical laws are often found subsequently to agree with the results of sophisticated modern precision measurements at the 9, 12 or 15 digit precision level. This lecture considers some precision laser interferometer and atomic beam experiments which might be suitable for detecting very small departures from the perfect spatial isotropy postulated in special relativity, as well as for more sensitively testing the basic Lorentz transformations.

*601,652*
**PB87-111647** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

**Limits for Spatial Anisotropy by Use of Nuclear-Spin-Polarized (9)Be(1+) Ions.**
Final rept.,
J. D. Prestage, J. J. Bollinger, W. M. Itano, and D. J. Wineland. 1985, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Physical Review Letters 54, n22 p2387-2390, 3 Jun 85.

Keywords: Atomic clocks, Hyperfine structure, Nuclear spin, Polarization(Spin alignment), Anisotropy, Reprints, *Beryllium ions, Beryllium 9, Hydrogen masers, Laser cooling, Hughes-Drever experiment.

The frequency of a nuclear spin-flip (/ Delta (m sub 1) / = 1) transition in (9)Be(1+) has been compared to the frequency of a hydrogen maser transition (/ Delta F / = 1. Delta (m sub F) = 0) to see if the relative frequencies depend on the orientation of the (9)Be(1+) ions in space. The present null result represents a decrease in the limits set by Hughes and Drever on a spatial anisotropy by a factor of about 300.

*601,653*
**PB87-114906** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Discussion on 81 WM 014-O 'Dielectric Strength of N2 - He Mixtures and Comparison with N2 - SF6 and CO2 - SF6 Mixtures' by J. M. Pelletier, Y. Gervais, and D. Mukhedkar.**
Final rept.,
R. J. Van Brunt. 1981, 2p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in Institute of Electrical and Electronics Engineers Transactions on Power Apparatus and Systems PAS-100, n8 p3867-3868 Aug 81.

Keywords: *Gas ionization, *Dielectric breakdown, Dielectric properties, Ideal gas law, Pressure, Comparison, Nitrogen, Helium, Carbon dioxide, Sulfur hexafluoride, Reprints, Paschen law, Olivier equation.

Comments are given concerning the limitations and applicability of Oliviers equation used by J. M. Pelletier, et al., to fit data on electrical breakdown for gas mixtures. A connection is drawn between Olivier's equation and Paschen's law, and the effect of deviations from ideal gas behavior at higher pressures is pointed out.

*601,654*
**PB87-116141** PC **A06**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
**Bibliography of Photon Total Cross Section (Attenuation Coefficient) Measurements 10 eV to 13.5 GeV,**
J. H. Hubbell, H. M. Gerstenberg, and E. B. Saloman. Oct 86, 104p NBSIR-86/3461
Sponsored by Department of Energy, Washington, DC., and Office of Naval Research, Arlington, VA.

Keywords: *Photon cross sections, *Far ultraviolet radiation, *X rays, *Gamma rays, *Bibliographies, Bremsstrahlung, Attenuation, *Absorption coefficients, *Total cross sections.

The authors present a bibliography of papers reporting absolute measurements of photon (XUV, x-ray, gamma-ray, bremsstrahlung) total interaction cross sections or attenuation coefficients for the elements and some compounds. The energy range covered is from 10 eV to above 10 GeV. The papers are part of the reference collection of the National Bureau of Standards Photon and Charged Particle Data Center. They cover the period from 1907 to March 1986. Included with each reference are annotations specifying the substances studied and the duplicative references to a total of about 20,000 data points. All these data are available in machine-readable form.

*601,655*
**PB87-117180** PC **A03**/MF **A01**
National Bureau of Standards, Gaithersburg, MD.
**Water Bath Blackbody for the 5 to 60C Temperature Range: Performance Goal, Design Concept, and Test Results.**
Final rept.,
J. Geist, and J. B. Fowler. Oct 86, 26p NBS/TN-1228
Also available from Supt. of Docs as SN003-003-02767-7. Errata sheet inserted. Sponsored by Aerospace Guidance and Metrology Center, Newark AFS, OH.

Keywords: *Blackbody radiation, *Standards, Performance, Design, Tests.

A water bath blackbody has been built under contract for the Electromagnetic Metrology Engineering Branch at Newark Air Force Station. The performance goal was a large-area, self-calibrating, high-accuracy blackbody covering the majority of the liquid water temperature range. With the exception of self-calibration, these goals were met. The report describes both the conceptual design of the water bath blackbody and the results of the tests that were carried out to characterize the performance of the actual water bath blackbody that was built for Newark Air Force Station. The details of the construction and operation of that water bath blackbody are described in a companion report.

*601,656*
**PB87-118113** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
**Comparison of Centrifugal and Fountain Effect Pumps.**
Final rept.,
V. Arp. 1986, 4p
Contract NASA-A-210590
Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center.
Pub. in Cryogenics 26, p103-106 Feb 86.

Keywords: *Centrifugal pumps, *Superfluidity, Liquid helium, Comparison, Efficiency, Helium 4, Reprints, *Fountain effect pumps, Helium II.

The efficiency of a pumping system is defined in terms of energy flows into and out of a control volume surrounding the pump. It is shown that the centrifugal pump power requirement is affected little by the heat leaks expected in a planned He II transfer system. In contrast, the power requirement for a superfluid fountain effect pump is greatly dependent on the thermal conduction through both the porous plug and the downstream transfer line. If the downstream conduction is negligible, the efficiency of a fountain effect pump will be significantly less than that of available centrifugal pumps.

*601,657*
**PB87-118709** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
**Measurement of the Ratio of the Speed of Sound to the Speed of Light.**
Final rept.,
J. B. Mehl, and M. R. Moldover. 1986, 4p
Physical Review A: General Physics 34, n4 p3341-3344 Oct 86.

Keywords: *Acoustic velocity, Temperature measurement, Ideal gas law, Ratios, Reprints, *Light speed.

Measurements of the resonance frequencies of the acoustic modes and of the microwave modes of a single cavity can determine u/c, the ratio of the speed of sound of a gas to the speed of light. Such measurements with a monatomic gas would determine the thermodynamic temperature T with unprecedented accuracy. By judicious choices of cavity geometry and resonance modes, u/c can be measured to part-per-million accuracy using cavities whose geometry is known only to parts per thousand. These techniques can also be applied to measurements of the universal gas constant R. A measurement of R would also require an accurate determination of the average atomic mass of the monatomic gas.

*601,658*
**PB87-118972** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Laser Manipulation of Atomic-Beam Velocities--Demonstration of Stopped Atoms and Velocity Reversal.**
Final rept.,
W. Ertmer, R. Blatt, J. L. Hall, and M. Zhu. 1985, 4p
Grant NSF-PHY82-00805, Contract N00014-77-C-0656
Sponsored by National Science Foundation, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in Physical Review Letters 54, n10 p996-999 1985.

Keywords: *Atomic beams, Reprints, *Laser cooling, Sodium atoms, Atom traps.

Successful modification of the velocity of atomic beam sodium atoms to zero or negative values are reported, by using counter-propagating laser radiation which has been frequency-chirped, using precise electro-optic modulation techniques. The resulting 'gas cloud' had a temperature below 50 milli-Kelvin and a density above one million atoms/cc. Some near future possibilities are considered in atom slowing, deflection, and storage.

*601,659*
**PB87-121315** PC **A04/MF A01**
National Bureau of Standards, Gaithersburg, MD.
**Journal of Research of the National Bureau of Standards, Volume 91, Number 5, September-October 1986.**
Bi-monthly rept.
Oct 86, 74p
See also PB87-121323 through PB87-121356, and PB87-100186. Also available from Supt. of Docs as SN703-027-00012-1.

Keywords: *Research, Near infrared radiation, Standards, Units of measurement, Calorimeters, Enthalpy, Combustion, Wavelength standards, Quantum Hall effect, Josephson effect, Volt, Ohm, Voltage standards, Resistance standards, Triple points, Solid wastes.

Table of contents includes the following: A wavelength standard for the near infrared based on the reflectance of rare-earth oxides; The triple point of oxygen in sealed transportable cells; A multi-kilogram capacity calorimeter for heterogeneous materials; Possible changes in the U.S. legal units of voltage and resistance.

*601,660*
**PB87-122438** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Corona Excited Supersonic Expansion.**
Final rept.,
P. C. Engelking. Sep 86, 4p
Pub. in Review of Scientific Instruments 57, n9 p2274-2277 Sep 86.

Keywords: *Ion sources, *Chemical radicals, *Electric corona, Free radicals, Supersonic flow, Plasma devices, Jets, Reprints.

Stable operation of a corona excited supersonic expansion for the production of cold radicals or ions requires control of the geometry, chemistry, and electrical parameters. The nozzle must taper rapidly on the high-pressure side to a throat that opens up into a free expansion on the vacuum side. Optimum radical and ion production is obtained with only a few percent of precursor in an inert carrier gas. Capacitive loading must be kept to a minimum to prevent oscillation. It is shown that the finite response time of the plasma synthesizes an inductance that serves to decouple the negative resistance of the plasma from the rest of the circuit. Practically, oscillation is prevented if the circuit RC time constant is shorter than that which the plasma can follow.

*601,661*
**PB87-128062** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Frequency Standards Based on Optically Pumped Cesium.**
Final rept.,
R. E. Drullinger. 1986, 3p
Pub. in Proceedings of the Institute of Electrical and Electronics Engineers 74, n1 p140-142 Jan 86.

Keywords: *Cesium frequency standards, *Standards, Atomic beams, Optical pumping, Reprints.

The state of development of optically pumped cesium-beam frequency standards is reviewed. The replacement of magnetic methods for atomic state selection and detection by optical (laser) methods provides potential for major reductions in systematic errors as well as a large increase in useable atomic beam flux. These translate to higher accuracy and better stability (both short and long term) or longer operating life if the beam current is reduced. With current technology it appears possible to construct a laboratory primary standard based on the concept. Simple and inexpensive field standards can also benefit from the optical pumping technology, but additional improvements in stabilized laser diodes will be needed.

*601,662*
**PB87-128187** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.
**Collective Excitation in the Crystalline Nucleus Model.**
Final rept.,
M. Danos, and A. Johnson. 1986, 4p
Pub. in Europhysics Letters 2, n3 p205-208 1986.

Keywords: *Nuclear models, Wave functions, Reprints, *Cluster model, Giant resonance.

In the paper the authors describe the mass dependence of the giant dipole resonance energy in terms of the crystalline model of the nucleus in which the alpha-particle is the basic unit. The experimental energies can be well reproduced for all nuclei heavier than the He nucleus. Because the success of the model depends on the correct counting of the relevant degrees of freedom, this result strongly suggests that four-particle correlations are an important aspect of the nuclear wave function.

*601,663*
**PB87-128336** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Losses in a Nb-Ti Superconductor as Functions of AC Field Amplitude and DC Transport Current.**
Final rept.,
M. Dragomirecky, J. V. Minervini, J. W. Ekin, R. B. Goldfarb, and A. F. Clark. 1986, 5p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Proceedings of International Cryogenic Engineering Conference (11th), Berlin (West Germany), April 22-25, 1986, p746-750.

Keywords: *Superconductors, Losses, Alternating current, Direct current, Magnetic fields, Electric current, Hysteresis, *Niobium titanium, Superconducting coils, Two-dimensional calculations.

Hysteretic shielding losses and transport losses were measured in a multifilamentary Nb-Ti superconducting coil as functions of transverse ac field amplitude and dc transport current. The conductor was biased with a dc field. There was significant agreement with the predictions of Minervini's two-dimensional theoretical model.

*601,664*
**PB87-128369** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**AC Losses in Nb-Ti Measured by Magnetization and Complex Susceptibility.**
Final rept.,
R. B. Goldfarb, and A. F. Clark. 1986, 8p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Advances in Cryogenic Engineering Materials 32, p779-786 1986.

Keywords: *Superconductors, Alternating current, Hysteresis, Losses, Magnetization, Magnetic fields, Direct current, *Foreign technology, *Niobium titanium, Magnetic susceptibility, Transients.

DC magnetization and complex ac susceptibility were measured at 4 K as functions of longitudinal dc field for a multifilamentary Nb-Ti superconductor with no transport current. Minor hysteresis loops were obtained in the dc measurements. The full-penetration field, H(p), a function of applied field, H, was deduced directly for each minor loop. The values for H(p) were fit to the Kim-type equation.

*601,665*
**PB87-128377** Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
**Effect of Aspect Ratio on Critical Current in Multifilamentary Superconductors.**
Final rept.,
L. F. Goodrich, W. P. Dube, E. S. Pittman, and A. F. Clark. 1986, 8p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Advances in Cryogenic Engineering Materials 32, p833-840 1986.

Keywords: *Superconductors, Magnetic fields, Niobium intermetallics, Tin intermetallics, Titanium intermetallics, Reprints, *Critical current, Niobium titanium, Niobium tin.

Experimental data and discussion are presented on the critical current of straight superconductors as a function of the orientation of a perpendicular applied magnetic field. Commercial, multifilamentary NbTi and Nb3Sn samples were measured in a radial access magnet that allowed an arbitrary angle setting. The change in critical current was measured at different magnetic fields to scale the effect for use in a standard test method. For a NbTi sample, the critical current with the magnetic field parallel to the wider face of the conductor is higher than that with the perpendicular orientation. The effect can be as high as 40% for a NbTi sample with an aspect ratio of six. The effect in Nb3Sn is opposite that in NbTi. A discussion of the most likely cause of the effect, which accounts for the difference between NbTi and Nb3Sn, is given.

*601,666*
**PB87-128385** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Shell-Model Interaction Energies in a Relativistic Hamiltonian Formulation (II).**
Final rept.,
M. Cauvin, V. Gillet, T. Kohmura, T. Suzuki, and M. Danos. 1986, 14p
Pub. in Nuclear Physics A456, p733-746 1986.

Keywords: Nuclear structure, Nuclear shell models, Degrees of freedom, Hamiltonian functions, Relativity, Reprints, *Nuclear forces.

The two-nucleon interaction energies of light and medium nuclei are discussed in a picture of mesonic degrees of freedom and a pure shell model for nucleons. The role of the different mesons in the interaction energies and the domain of the best values of the coupling constants are explored by calculating the mean square deviation between theoretical and experimental two-nucleon interaction energies. Because of the redundancies between different meson contributions to the interaction energies, the values of the coupling constants are not uniquely determined, and rather large domains of best values are obtained. These domains include sets of values of the coupling constants which are compatible with those from other sources. The experimental data can be reproduced with the same quality as in conventional phenomenological potential models by taking the meson fields, sigma, pi, rho, and omega, and using only vector coupling for the vector fields.

*601,667*
**PB87-131876** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
**Electro-Optic Field Measurement at a Needle Tip and Streamer Initiation in Nitrobenzene.**
Final rept.,
E. F. Kelley, and R. E. Hebner. 1986, 6p
Sponsored by Department of Energy, Washington, DC. Office of Energy Systems Research.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) 1986 Annual Report - Proceedings of Conference on Electrical Insulation and Dielectric Phenomena, Claymont, DE., November 3-6, 1986, p272-277.

Keywords: *Electrooptics, *Nitrobenzenes, *Electric discharges, Kerr electrooptical effect, High speed photography, Aromatic hydrocarbons, Streamer initiation.

Kerr-effect electro-optic observations of the impulse field are made in the vicinity of the tip of a needle-sphere electrode geometry. Distortions from the Laplacian field indicate charge injection from the tip along a narrow channel prior to streamer initiation. Estimates reveal charge densities of order 100 micro C/cc exists in the channel. An order of magnitude calculation suggests sufficient energy is deposited in the channel to cause vaporization of the liquid due to joule heating. The streamer will initiate where the charge injection channel touches the electrode.

*601,668*
**PB87-132221** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

**Particle-Hole Symmetry in the Interacting-Boson Model: Fermion and Boson Aspects.**
Final rept.,
A. B. Johnson, and C. M. Vincent. 1985, 6p
Grant NSF-THY82-13597
Sponsored by National Research Council, Washington, DC.
Pub. in Physical Review C: Condensed Matter 31, n4 p1540-1545 Apr 85.

Keywords: *Nuclear structure, Nuclear shell models, Bosons, Fermions, Reprints, Collective model.

It is shown that the S-D subspaces, which are used in the OAI microscopic derivation of the interacting boson model, form a particle-hole-symmetric family. Consequently there exist particle-hole-symmetric prescriptions for determining the structure of the S and D pairs. The result does not (as stated by Talmi) require the Hamiltonian to conserve generalized seniority. Nevertheless there are derivations from particle-hole symmetry when boson matrix elements involving more than two d bosons are calculated in lowest order using the boson mapping procedure of Otsuka, Arima, and Iachello. These deviations are used to estimate the inaccuracies introduced by the lowest-order mapping.

*601,669*
**PB87-134227** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
**Atomic-Beam Cooling: A Simulation Approach.**
Final rept.,
R. Blatt, W. Ertmer, P. Zoller, and J. L. Hall. 1986, 12p
Grants N000014-77-A-0016, NSF-PHY82-00805
Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in Physical Review A: General Physics 34, n4 p3022-3033 Oct 86.

Keywords: *Atomic beams, Mathematical models, Computerized simulation, Reprints, *Laser cooling.

Laser cooling of atoms in an atomic beam is studied theoretically by using a simulation approach derived from a pure-state analysis of resonant radiation pressure. Detailed numerical results are presented discussing the form of the atomic velocity distribution (and its minimum achievable width) and effects due to the spatial (focusing) and frequency variation of a Gaussian laser beam. A comparison of these results with recent experiments is given.

*601,670*
**PB87-134847** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Absorption and Scattering of Photons by the Delta Resonance.**
Final rept.,
E. Hayward. 1985, 11p
Pub. in AIP (American Institute of Physics) Conference Proceedings on Capture Gamma-Ray Spectrosc. Relat. Top. 125, p131-141 1985.

Keywords: *Photonuclear reactions, Absorption cross sections, Scattering cross sections, Gamma rays, Reprints, N star resonances, Sum rules.

Recently, the experiments on the total photonuclear absorption cross sections have been extended to encompass the Delta resonance in complex nuclei. These important experiments involve at least four different techniques and have been performed in European Laboratories. These results are compared with the total cross sections measured in the giant resonance region and extending up to the meson threshold. The Gell-Mann-Goldberger-Thirring sum provides a connection between the absorption cross sections in these two energy regions and the photo pion cross sections of the nucleon. The total photonuclear absorption cross sections are related to the forward coherent scattering cross sections through the optical theorem and dispersion relation. At backward angles, where measurements are possible, the scattering cross sections are strongly depressed by a form factor. The experimental cross sections do, however, exceed the prediction of a simple model.

*601,671*
**PB87-134854** Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Lorentz Transformations.**
Final rept.,
R. W. Hayward. 1985, 4p
Pub. in Encyclopedia of Physics, 3rd Edition, p666-669 1985.

Keywords: *Lorentz transformations, Elementary particles, Electromagnetism, Parity, Minkowski space, Light speed, Space-time, Conservation laws.

Lorentz transformations are defined in terms of rotations and velocity boosts in Minkowski space of the space-time coordinates or of the physical object. The physical meaning of orbital and spin angular momentum appears.

*601,672*
**PB87-134953** Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
**Frequency Standard Research Using Stored Ions.**
Final rept.,
D. J. Wineland, W. M. Itano, J. C. Bergquist, J. J. Bollinger, and H. Hemmati. 1984, 4p
Pub. in Progress in Quantum Electronics 8, p139-142 1984.

Keywords: *Frequency standards, Atomic clocks, Atomic spectroscopy, Reprints, Ion storage, Laser spectroscopy.

The authors summarize research undertaken to develop time and frequency standards based on stored ions. The ion storage method for high resolution spectroscopy is also briefly compared to the methods for stored neutrals and slow atomic beams.

*601,673*
**PB87-140315** PC **A15**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
**Technical Activities 1986, Center for Basic Standards,**
P. L. M. Heydemann. Oct 86, 340p NBSIR-86/3469
See also PB86-140043.

Keywords: *Research, *Standards, Metrology, Fundamental constants, Pressure, Vacuum, Electrical measurement, Temperature, Atomic physics, Frequency standards, Gravity, X rays, Gamma rays, Laser applications.

The report summarizes the research and technical activities of the Center for Basic Standards during the Fiscal Year 1986. These activities include work in the areas of electricity, temperature and pressure, mass and length, time and frequency, quantum metrology, and quantum physics.

# SPACE TECHNOLOGY

## Manned Spacecraft

*601,674*
**PB87-103305** PC **A03**/MF **A01**
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
**Transport of Electrons and Associated Bremsstrahlung Through a Composite Aluminum-Lead Shield, with Applications to Spacecraft Shielding,**
G. Barnea, S. M. Seltzer, and M. J. Berger. Jul 86, 28p NBSIR-86/3429
Sponsored by Department of Energy, Washington, DC. Office of Health and Environmental Research, and Office of Naval Research, Arlington, VA.

Keywords: *Electron irradiation, *Bremsstrahlung, *Radiation shielding, Monte Carlo method, *Spacecraft shielding.

Monte Carlo calculations have been made of the stopping of electrons and the penetration of secondary bremsstrahlung through layered aluminum-lead spacecraft walls. The results are presented in terms of the resultant radiation dose to objects inside. Dose values for monoenergetic incident electrons are given as a function of the aluminum/lead thickness ratio. These data, integrated over a few typical earth-orbit electron spectra, demonstrate the substantial reduction in radiation dose that can be achieved by replacing a portion of an aluminum shield with an inner layer of lead. The main results were obtained by applying a complex-geometry code to spherical-shell configurations. It was found that these results could be reasonably well approximated by an alternative and more economical approach, involving the use of slab-geometry transport results.

# TRANSPORTATION

## Pipeline Transportation

*601,675*
**PB87-108189** Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Fracture and Deformation Div.
**Handling Blunt Flaws in a Fitness-for-Service Assessment of Pipeline Weld Quality.**
Final rept.,
M. B. Kasen, and G. E. Hicho. 1986, 10p
See also PB86-162039. Sponsored by Department of Transportation, Washington, DC. Office of Pipeline Safety Operations.
Pub. in the International Conference and Exposition on Fatigue, Corrosion Cracking, Fracture Mechanics, and Failure Analysis, Salt Lake City, UT., December 2-6, 1985, p295-304 1986.

Keywords: *Pipelines, *Welded joints, Quality, Crack propagation, Slags, Porosity, Fatigue(Materials), Fractures(Materials), Inspection, Defects.

The significance of porosity, slag and arc burns on pipeline integrity is evaluated by assessing the probability of their contributing to crack initiation and to accel erated crack growth during low cycle fatigue.

## Transportation Safety

*601,676*
**PB86-163524** Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
**Role of Aircraft Panel Materials in Cabin Fires and Their Properties.**
Final rept.,
J. Quintiere, V. Babrauskas, L. Cooper, M. Harkleroad, and K. Steckler. Jun 85, 109p
Sponsored by National Aviation Facilities Experimental Center, Atlantic City, NJ.
Pub. in DOT/FAA/CT-84/30, 109p 1985.

Keywords: *Aircraft cabins, *Fires, Combustion, Flammability, Heat transfer, Ignition, Reprints.

The report examines the fire development in the FAA C 133 post crash fire experiments involving a fully furnished cabin section. In particular the rate and involvement of aircraft wall and ceiling panels are examined. For two full-scale experiments the energy release rate of the interior cabin furnishings were estimated and an estimate of ceiling ignition computed. Also flammability data on ignition, combustion, and heat transfer at various external irradiance, for one device at diminished ambient oxygen, were compiled from several test apparatuses for five candidate aircraft panel materials.

# URBAN & REGIONAL TECHNOLOGY & DEVELOPMENT

## Fire Services, Law Enforcement, & Criminal Justice

*601,677*
**PB86-213089** PC **A04**/MF **A01**

National Bureau of Standards (NEL), Gaithersburg, MD. Law Enforcement Standards Lab.
**Directory of Law Enforcement and Criminal Justice Associations and Research Centers, 1985 Edition.**
Special pub.,
S. Lyles. Apr 86, 58p NBS/SP-480/20-1985
Supersedes PB-279246. Sponsored by National Inst. of Justice, Washington, DC.

Keywords: *Directories, *Law enforcement, *Laboratories, *Organizations, User needs, United States, Communication equipment, Security systems, Protective clothing, Criminal justice, Investigative aids.

The Law Enforcement Standards Laboratory (LESL) of the National Bureau of Standards (NBS) furnishes technical support to the National Institute of Justice (NIJ) program to strengthen law enforcement and criminal justice in the United States. LESL's function is to conduct research that will assist law enforcement and criminal justice agencies in the selection and procurement of quality equipment. The document is a law enforcement equipment report developed by LESL under the sponsorship of NIJ as part of the Technology Assessment Program, which is described on page iv. Additional reports as well as other documents are being issued under the LESL program in the areas of protective equipment, communications equipment, security systems, weapons, emergency equipment, investigative aids, vehicles, and clothing.

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2s(2) 2p(5) - 2s 2p(6) Transitions in Fluorinelike Ions from Zr(31+ ) to SN(41+ ).
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4d-Photoabsorption of Barium: A View of Shell Collapse vs Contraction.
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10-60 GHz G/T Measurements Using the Sun as a Source--A Preliminary Study.
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130 MM (5.25 in) Flexible Disk Cartridge Track Format Using Modified Frequency Modulation Recording at 7958 BPRAD on Two Sides - 1.9 TPMM (48 TPI) for Information Interchange. Category: Hardware Standard. Subcategory: Interchange Codes and Media.
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PB87-136644 *601,491* PC **A19**/MF **A01**

**PB87-136651**
Prediction of the Long Term Stability of Polyester-Based Recording Media,
PB87-136651 *601,286* PC **A08**/MF **A01**

**PB87-136669**
Technical Activities 1986, Center for Chemical Physics,
PB87-136669 *600,613* PC **A16**/MF **A01**

**PB87-136677**
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PB87-136677 *601,058* PC **A07**/MF **A01**

**PB87-136685**
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**PB87-136693**
Institute for Materials Science and Engineering, Polymers: Technical Activities 1986.
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**PB87-136701**
Institute for Materials Science and Engineering, Fracture and Deformation: Technical Activities 1986.
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**PB87-137162**
Temperature Dependence of Spectral Broadening in the Hg (6 singlet S(sub 0) - 6 triplet P(sub 1) Multiplet at High Optical Densities,
PB87-137162 *600,220*
(Order as PB87-137154, PC **A04**/MF **A01**)

**PB87-137170**
Absolute Isotopic Abundance Ratio and Atomic Weight of a Reference Sample of Gallium,
PB87-137170 *600,276*
(Order as PB87-137154, PC **A04**/MF **A01**)

**PB87-137188**
Thermal Expansion of Platinum and Platinum-Rhodium Alloys,
PB87-137188 *600,614*
(Order as PB87-137154, PC **A04**/MF **A01**)

**PB87-138376**
Strain Energy of Bituminous Built-Up Membranes: An Alternative to the Tensile Strength Criterion,
PB87-138376 *600,124* PC **A04**/MF **A01**

**PB87-138384**
Design of the National Bureau of Standards Isotropic Magnetic Field Meter (MFM-10) 300 kHz to 100 MHz,
PB87-138384 *600,877* PC **A04**/MF **A01**

**PB87-140141**
Fluid-Structure Interaction Effects for Offshore Structures.
PB87-140141 *601,416* PC **A04**/MF **A01**

**PB87-140174**
Nondestructive Evaluation Activities in the Semiconductor Materials and Processes Division,

PB87-140174 *601,564* PC **A03**/MF **A01**

**PB87-140182**
Calculated Interaction of Water Droplet Sprays with Fire Plumes in Compartments.
PB87-140182 *600,145* PC **A03**/MF **A01**

**PB87-140190**
Fire Propagation in Concurrent Flows.
PB87-140190 *600,682* PC **A04**/MF **A01**

**PB87-140208**
Towards a Theory for the Orientation Dependent Packing Entropy of Inhomogeneous Polymer Systems,
PB87-140208 *600,641* PC **A04**/MF **A01**

**PB87-140216**
Building Technology Project Summaries 1986,
PB87-140216 *600,146* PC **A04**/MF **A01**

**PB87-140224**
Technical Activities 1986, Molecular Spectroscopy Division,
PB87-140224 *600,221* PC **A06**/MF **A01**

**PB87-140232**
Technical Activities 1986, Center for Radiation Research,
PB87-140232 *600,277* PC **A14**/MF **A01**

**PB87-140240**
Prediction of Fire Properties of Materials. Part 1. Aliphatic and Aromatic Hydrocarbons and Related Polymers.
PB87-140240 *600,683* PC **A04**/MF **A01**

**PB87-140257**
Time-Dependent Simulation of Small-Scale Turbulent Mixing and Reaction.
PB87-140257 *600,684* PC **A03**/MF **A01**

**PB87-140265**
Comparison of the Toxicity of the Combustion Products from a Flexible Polyurethane Foam and a Polyester Fabric Evaluated Separately and Together by the NBS (National Bureau of Standards) Toxicity Test Method and a Cone Radiant Heater Toxicity Test Apparatus,
PB87-140265 *601,365* PC **A04**/MF **A01**

**PB87-140273**
Technical Publication Announcements Covering Center Programs, January to March 1986,
PB87-140273 *600,878* PC **A02**/MF **A01**

**PB87-140281**
Tiletool: A Graphical Interface for the Exploration of Generalized Penrose Tilings,
PB87-140281 *600,695* PC **A02**/MF **A01**

**PB87-140299**
Application of Smoke Detector Technology to Quantitative Respirator Fit Test Methodology.
PB87-140299 *600,066* PC **A04**/MF **A01**

**PB87-140307**
Cobalt-60 Facilities Available for Hardness Assurance Testing.
PB87-140307 *600,834* PC **A03**/MF **A01**

**PB87-140315**
Technical Activities 1986, Center for Basic Standards,
PB87-140315 *601,673* PC **A15**/MF **A01**

**PB87-140414**
Crystal Data: Version 1.0 Database Specifications.
PB87-140414 *601,565* PC **A04**/MF **A01**

**PB87-140422**
Handbook for the Quality Assurance of Meteorlogical Measurements.
PB87-140422 *600,052* PC **A13**/MF **A01**

**PB87-140570**
Computer Code for Gas-Liquid Two-Phase Vortex Motions: GLVM,
PB87-140570 *600,615* PC **A03**/MF **A01**

**PB87-140588**
DOE/NBS (Department of Energy/National Bureau of Standards) Forum on Testing and Rating Procedures for Consumer Products, October 2-3, 1985.
PB87-140588 *600,148* PC **A04**/MF **A01**

**PB87-140596**
B2DE - A Program for Solving Systems of Partial Differential Equations in Two Dimensions,
PB87-140596 *601,301* PC **A04**/MF **A01**

**PB87-140604**
Cost Comparison of Selected Alternatives for Preserving Historic Pension Files.
PB87-140604 *601,072* PC **A04**/MF **A01**

**PB87-140729**
Handbook for Operation and Maintenance of an NBS (National Bureau of Standards) Multisensor Automated EM (Electromagnetic) Field Measurement System.
PB87-140729 *600,879* PC **A04**/MF **A01**

**PB87-140810**
Guidance on Software Package Selection.
PB87-140810 *600,742* PC **A06**/MF **A01**

**PB87-141487**
Natural Gas Handbook,
PB87-141487 *600,901* PC **A06**/MF **A01**

**PB87-142436**
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PB87-142436 *600,755* CP **T05**

**PB87-145058**
Statistical Characterization of Electroexplosive Devices Relevant to Electromagnetic Compatibility Assessment.
PB87-145058 *601,417* PC **A04**/MF **A01**

**PB87-145066**
Interactive FORTRAN Programs for Micro Computers to Calculate the Thermophysical Properties of Twelve Fluids (MIPROPS).
PB87-145066 *600,616* PC **A05**/MF **A01**

**PB87-145272**
Publications of the National Bureau of Standards, 1985 Catalog.
PB87-145272 *601,109* PC **A17**/MF **A01**

**PB87-145371**
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PB87-145371 *600,617* Not available NTIS

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Measuring the Corrosion Rate of Reinforcing Steel Concrete - Final Report,
PB87-145413 *600,662* PC **A03**/MF **A01**

**PB87-145421**
Transient Cooling of a Hot Surface by Droplets Evaporation. Final Report.,
PB87-145421 *600,970* PC **A07**/MF **A01**

**PB87-148300**
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PB87-148300 *600,618* Not available NTIS

**PB87-148318**
Improved International Formulations for the Viscosity and Thermal Conductivity of Water Substance,
PB87-148318 *600,619* Not available NTIS

**PB87-148326**
Viscosity and Thermal Conductivity of Normal Hydrogen in the Limit of Zero Density,
PB87-148326 *600,620* Not available NTIS

**PB87-148334**
Viscosity and Thermal Conductivity Coefficients of Gaseous and Liquid Argon,
PB87-148334 *600,621* Not available NTIS

**PB87-148342**
Standard Chemical Thermodynamic Properties of Alkyne Isomer Groups,
PB87-148342 *600,622* Not available NTIS

**PB87-148359**
Recent Progress in Deuterium Triple-Point Measurements,
PB87-148359 *600,623* Not available NTIS

**PB87-148367**
Rate Constants for Reactions of Radiation-Produced Transients in Aqueous Solutions of Actinides,
PB87-148367 *600,278* Not available NTIS

**PB87-148375**
Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C1 to C4. Part 2. Ideal Gas Properties,
PB87-148375 *600,624* Not available NTIS

**PNL-SA-12071**
Monte Carlo Calculation of Energy Deposition and Ionization Yield for High Energy Protons.
DE85005518 *601,403* PC **A02**/MF **A01**

**REPT-86-7**
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PB87-145421 *600,970* PC **A07**/MF **A01**

**SBI-AD-F300-488**
Electronic Typesetting Program Programmer's Manual.
AD-A147 500/3 *600,694* PC **A07**/MF **A01**

**SLAC-PUB-3697**
FASTBUS for the Particle Accelerator Laboratories.
DE85014352 *601,391* PC **A02**/MF **A01**

**TR-21**
Rigorous Bounds for the Calculated Dielectric Constants of Ferroelectric Polymers.
AD-A132 741/0 *600,281* PC **A02**/MF **A01**

**TR-82-1**
Acoustic Emission Transducer Calibration by Means of the Seismic Surface Pulse.
AD-A148 921/0 *601,421* PC **A02**/MF **A01**

**UCRL-88533**
Mechanism of the Optogalvanic Effect in a Hollow-Cathode Discharge.
DE83013583 *600,287* PC **A02**/MF **A01**

# APPENDIX A
# List of Depository Libraries in the United States

## ALABAMA

### Alexander City

Alexander City State Junior College Thomas S. Russell Library (1967)*

### Auburn

Auburn University Ralph Brown Draughon Library (1907)

### Birmingham

Birmingham Public Library (1895)
Birmingham-Southern College Library (1932)
Jefferson State Junior College James B. Allen Library (1970)
Miles College C. A. Kirkendoll Learning Resource Center (1980)
Samford University Library (1884)

### Enterprise

Enterprise State Junior College Learning Resources Center (1967)

### Fayette

Brewer State Junior College Learning Resources Center Library (1979)

### Florence

University of North Alabama Collier Library (1932)

### Gadsden

Gadsden Public Library (1963)

### Huntsville

University of Alabama in Huntsville Library (1964)

### Jacksonville

Jacksonville State University Houston Cole Library (1929)

### Mobile

Mobile Public Library (1963)
Spring Hill College Thomas Byrne Memorial Library (1937)
University of South Alabama Library (1968)

### Montgomery

Alabama Public Library Service (1984)
Alabama Supreme Court and State Law Library (1884)
Auburn University at Montgomery Library (1971) REGIONAL
Air University Library Maxwell Air Force Base (1963)

### Normal

Alabama Agricultural and Mechanical University J. F. Drake Memorial Learning Resources Center (1963)

### Troy

Troy State University Library (1963)

### Tuskegee Institute

Tuskegee Institute Hollis Burke Frissell Library (1907)

### University

University of Alabama Library (1860) REGIONAL
University of Alabama School of Law Library (1967)

## ALASKA

### Anchorage

Anchorage Law Library (1973)
Anchorage Municipal Libraries Z. J. Loussac Public Library (1978)
University of Alaska at Anchorage Library (1961)
U.S. Department of Interior Alaska Resources Library (1981)
U.S. District Court Library (1983)

### Fairbanks

University of Alaska Elmer E. Rasmuson Library (1922)

### Juneau

Alaska State Library (1900)
University of Alaska-Juneau Library (1981)

### Ketchikan

Ketchikan Community College Library (1970)

## AMERICAN SAMOA

### Pago Pago

Community College of American Samoa Library (1985)

*Year designated.

## ARIZONA

### Coolidge

Central Arizona College (1973)

### Flagstaff

Northern Arizona University Library (1937)

### Holbrook

Northland Pioneer College (1985)

### Mesa

Mesa Public Library (1983)

### Phoenix

Department of Library Archives, and Public Records (unknown) REGIONAL
Grand Canyon College Fleming Library (1978)
Phoenix Public Library (1917)
U.S. Court of Appeals (1984)

### Prescott

Yavapai College Library (1976)

### Tempe

Arizona State University College of Law Library (1977)
Arizona State University Library (1944)

### Tucson

Tucson Public Library (1970)
University of Arizona Library (1907) REGIONAL

### Yuma

Yuma City-County Library (1963)

## ARKANSAS

### Arkadelphia

Ouachita Baptist University Riley Library (1963)

### Batesville

Arkansas College Library (1963)

### Clarksville

College of the Ozarks Dobson Memorial Library (1925)

### Conway

Hendrix College Olin C. Bailey Library (1903)

### Fayetteville

University of Arkansas Mullins Library (1907)
University of Arkansas School of Law Library (1978)

### Little Rock

Arkansas State Library (1978) REGIONAL
Arkansas Supreme Court Library (1962)
Little Rock Public Library (1953)
University of Arlansas at Little Rock Library (1973)
University of Arkansas at Little Rock, School of Law Library (1979)

### Magnolia

Southern Arkansas University Magale Library (1956)

### Monticello

University of Arkansas at Monticello Library (1956)

### Pine Bluff

University of Arkansas at Pine Bluff Watson Memorial Library (1976)

### Russellville

Arkansas Tech University Tomlinson Library (1925)

### Searcy

Harding University Beaumont Memorial Library (1963)

### State University

Arkansas State University Dean B. Ellis Library (1913)

### Walnut Ridge

Southern Baptist College Felix Goodson Library (1967)

## CALIFORNIA

### Anaheim

Anaheim Public Library (1963)

### Arcadia

Arcadia Public Library (1975)

### Arcata

Humboldt State University Library (1963)

### Bakersfield

California State College Bakersfiedl Library (1974)
Kern County, Beale Memorial Library (1943)

### Berkeley

University of California General Library (1907)
University of California Law Library (1963)

### Carson

California State University Dominguez Hills Educational Resources Center (1973)
Carson Regional Library (1973)

### Chico

California State University Merriam Library (1962)

### Claremont

Claremont Colleges' Libraries Honnold Library (1913)

### Compton

Compton Public Library (1972)

### Culver City

Culver City Library (1966)

### Davis

University of California Shields Library (1953)
University of California at Davis Law Library (1972)

### Downey

Downey City Library (1963)

### Fresno

California State University, Fresno, Henry Madden Library (1962)
Fresno County Free Library (1920)

### Fullerton

California State University at Fullerton Library (1963)
Western State University College of Law Library (1984)

### Garden Grove

Garden Grove Regional Library (1963)

### Gardena

Gardena Public Library (1966)

### Hayward

California State University at Hayward Library (1963)

### Huntington Park

Huntington Park Library (1970)

### Inglewood

Inglewood Public Library (1963)

### Irvine

University of California at Irvine General Library (1963)

### La Jolla

University of California at San Deigo Central University Library (1963)

### Lakewood

Angelo Iacoboni Public Library (1970)

### Lancaster

Lancaster Library (1967)

### La Verne

University of La Verne College of Law Library (1979)

### Long Beach

California State University at Long Beach Library (1962)
Long Beach Public Library (1933)

### Los Angeles

California State University at Los Angeles John F. Kennedy Memorial Library (1956)
Los Angeles County Law Library (1963)
Los Angeles Public Library (1891)
Loyola Marymount University Charles Von der Ahe Library (1933)
Loyola Law School Law Library (1979)
Occidental College Library (1941)
Southwestern University School of Law Library (1975)
University of California, University Research Library (1932)
University of California, Los Angeles Law Library (1958)
University of Southern California Doheny Memorial Library (1933)
University of Southern California Law Library (1978)
U.S. Court of Appeals 9th Circuit Library (1981)
Whittier College School of Law Library (1978)

### Malibu

Pepperdine University Payson Library (1963)

### Menlo Park

Department of Interior Geological Survey Library (1962)

### Montebello

Montebello Regional Library (1966)

### Monterey

U.S. Naval Postgraduate School Dudley Knox Library (1963)

### Monterey Park

Bruggemeyer Memorial Library (1964)

### Northridge

California State University at Northridge, Oviatt Library (1958)

### Norwalk

Norwalk Regional Library (1973)

### Oakland

Mills College Library (1966)
Oakland Public Library (1923)

### Ontario

Ontario City Library (1974)

### Palm Springs

Palm Springs Public Library (1980)

### Pasadena

California Institute of Technology Millikan Memorial Library (1933)
Pasadena Public Library (1963)

### Pleasant Hill

Contra Costa County Library (1964)

### Redding

Shasta County Library (1956)

### Redlands

University of Redlands Armacost Library (1933)

### Redwood City

Redwood City Public Library (1966)

### Reseda

West Valley Regional Branch Library (1966)

### Richmond

Richmond Public Library (1943)

### Riverside

Riverside City and County Public Library (1947)
University of California at Riverside Library (1963)

### Sacramento

California State Library (1895) REGIONAL
California State University at Sacramento Library (1963)
Sacramento County Law Library (1963)
Sacramento Public Library (1880)
University of the Pacific McGeorge School of Law Library (1978)

### San Bernardino

San Bernardino County Law Library (1984)
San Bernardino County Library (1964)

### San Diego

San Diego County Law Library (1973)
San Diego County Library (1966)
San Diego Public Library (1895)
San Diego State University Library (1962)
University of San Diego Kratter Law Library (1967)

### San Francisco

Golden Gate University School of Law Library (1979)
Hastings College of Law Library (1972)
San Francisco Public Library (1889)
San Francisco State University J. Paul Leonard Library (1955)
Supreme Court of California Library (1979)
U.S. Court of Appeals Ninth Circuit Library (1971)
University of San Francisco Richard A. Gleeson Library (1963)

### San Jose

San Jose State University Library (1962)

### San Leandro

San Leandro Community Library Center (1961)

### San Luis Obispo

California Polytechnic State University Robert E. Kennedy Library (1969)

### San Rafael

Marin County Free Library (1975)

### Santa Ana

Orange County Law Library (1975)
Santa Ana Public Library (1959)

### Santa Barbara

University of California at Santa Barbara Library (1960)

### Santa Clara

University of Santa Clara Orradre Library (1963)

### Santa Cruz

University of California at Santa Cruz McHenry Library (1963)

### Santa Rosa

Sonoma County Library (1896)

### Stanford

Stanford University Libraries (1895)
Stanford University Robert Crown Law Library (1978)

### Stockton

Public Library of Stockton and San Joaquin County (1884)

### Thousand Oaks

California Lutheran College Library (1964)

### Torrance

Torrance Public Library (1969)

### Turlock

California State College Stanislaus Library (1964)

### Vallejo

Solano County Library, John F. Kennedy Library (1982)

### Valencia

Valencia Regional Library (1972)

### Ventura

Ventura County Library Services Agency (1975)

### Visalia

Tulare County Free Library (1967)

### Walnut

Mount San Antonio College Library (1966)

### West Covina

West Covina Regional Library (1966)

### Whittier

Whittier College Wardman Library (1963)

## CANAL ZONE

### Balboa Heights

Panama Canal Commission (1963)

## COLORADO

### Alamosa

Adams State College Library (1963)

### Aurora

Aurora Public Library (1984)

### Boulder

University of Colorado at Boulder Norlin Library (1879) REGIONAL

### Colorado Springs

Colorado College Tutt Library (1880)
University of Colorado at Colorado Springs Library (1974)
U.S. Air Force Academy Academy Library (1956)

### Denver

Auraria Library (1978)
Colorado State Library (unknown)
Colorado Supreme Court Library (1978)
Denver Public Library (1884) REGIONAL
Department of the Interior Bureau of Reclamation Library (1962)
Regis College Dayton Memorial Library (1915)
U.S. Court of Appeals Tenth Circuit Library (1973)
University of Denver Penrose Library (1909)
University of Denver College of Law Westminster Law Library (1978)

### Fort Collins

Colorado State University Libraries (1907)

### Golden

Colorado School Mines Arthur Lakes Library (1939)

### Grand Junction

Mesa College Lowell Heiny Library (1978)

### Greeley

University of Northern Colorado James A. Michener Library (1966)

### Gunnison

Western State College Leslie J. Savage Library (1932)

### La Junta

Otero Junior College Wheeler Library (1963)

### Lakewood

Jefferson County Public Library Lakewood Library (1968)

### Pueblo

Pueblo Library District (1893)
University of Southern Colorado Library (1965)

## CONNECTICUT

### Bridgeport

Bridgeport Public Library (1884)
University of Bridgeport School of Law Library Wahlstrom Library (1979)

### Danbury

Western Connecticut State University Ruth A. Haas Library (1967)

### Danielson

Quinebaug Valley Community College Audrey P. Beck Library (1975)

### Enfield

Enfield Central Library (1967)

### Hartford

Connecticut State Library (unknown) REGIONAL
Hartford Public Library (1945)
Trinity Collebe Library (1895)
University of Connecticut School of Law Library (1978)

### Middletown

Wesleyan University Olin Library (1906)

### Mystic

Mystic Seaport Museum, Incorporated G. W. Blunt White Library (1964)

### New Britain

Central Connecticut State University Elihu Burritt Library (1973)

### New Haven

Southern Connecticut State University Hilton C. Buley Library (1968)
Yale Law Library (1981)
Yale University Seeley G. Mudd Library (1859)

### New London

Connecticut College C. E. Shain Library (1926)
U.S. Coast Guard Academy Library (1939)

### Stamford

Ferguson Library (1973)

### Storrs

University of Connecticut Homer Babbidge Library (1907)

### Waterbury

Post College Traurig Library (1977)
Silas Bronson Public Library (1869)

### West Haven

University of New Haven Peterson Library (1971)

## DELAWARE

### Dover

Delaware State College William C. Jason Library (1962)
State Law Library in Kent County (unknown)

### Georgetown

Delaware Technical and Community College Library (1968)
Sussex County Law Library (1976)

### Newark

University of Delaware Library (1907)

### Wilmington

Delaware Law School Library (1976)
New Castle County Law Library (1974)

## DISTRICT OF COLUMBIA

### Washington

Administrative Conference of the United States Library (1972)
Advisory Commission on Intergovernmental Relations Library (1977)
American University Washington College of Law Library (1983)
Antioch School of Law Library (1982)
Catholic University of America Robert J. White Law Library (1979)
Department of the Army Pentagon Library ANRAL(1969)
Department of Commerce Library (1955)
Department of Health and Human Services Library (1954)
Department of Housing and Urban Development Library (1969)
Department of the Interior Library Natural Resources Library (1895)
Department of Justice Main Library (1895)
Department of Labor Library (1976)
Department of the Navy Library (1895)
Department of State Library (1895)
Department of State Law Library (1966)
Department of Transportation Main Library (1982)
Department of Transportation, U.S. Coast Guard Law Library (1982)
Department of the Treasury Library (1895)
District of Columbia Court of Appeals Library (1981)
District of Columbia Public Library (1943)
Equal Employment Opportunity Commission Library (1984)
Executive Office of the President, Office of Administration, Library & Information Service Division (1965)
Federal Deposit Insurance Corporation Library (1972)
Federal Election Commission Library (1975)
Federal Energy Regulatory Commission Library (1983)
Federal Labor Relations Authority Law Library (1982)
Federal Mine Safety & Health Review Commission Library (1979)
Federal Reserve System Board of Governors Research Library (1978)
Federal Rserve System Law Library (1976)
General Accounting Office Library (1974)
General Services Administration Library (1975)
Georgetown University Library (1969)
Georgetown University Law Center Fred O. Dennis Law Library (1978)
George Washington University Melvin Gelman Library (1983)
George Washington University National Law Center Jacob Burns Law Library (1978)
Library of Congress Congressional Research Service (1978)
Library of Congress Serial and Government Publications (1977)
Merit Systems Protection Board Library (1979)
National Defense University Library (1895)
Pension Benefit Guaranty Corporation Legal Dept. Library (1984)
U.S. Court of Appeals Judges' Library (1975)
U.S. Information Agency Library (1984)
U.S. Office of Personnel Management Library (1963)
U.S. Postal Service Library (1895)
U.S. Senate Library (1979)
U.S. Supreme Court Library (1978)
University of the District of Columbia Library (1970)
Verterans' Administration Central Office Library (1967)

## FLORIDA

### Boca Raton

Florida Atlantic University S. E. Wimberly Library (1963)

### Clearwater

Clearwater Public Library (1972)

### Coral Gables

University of Miami Library Otto G. Richter Library (1939)

### Daytona Beach

Volusia County Library Center (1963)

### De Land

Stetson University duPont-Ball Library (1887)

### Fort Lauderdale

Broward County Main Library (1967)
Nova University, Center for Study of Law/Law Library (1967)

### Fort Pierce

Indian River Comunity College Library (1975)

### Gainesville

University of Florida College of Law Library (1978)
University of Florida Libraries (1907) REGIONAL

### Jacksonville

Haydon Burns Public Library (1914)
Jacksonville University Swisher Library (1962)
University of North Florida Thomas G. Carpenter Library (1972)

### Lakeland

Lakeland Public Library (1928)

### Leesburg

Lake-Sumter Community College Library (1963)

### Melbourne

Florida Institute of Technology Library (1963)

### Miami

Florida International University Library (1970)
Miami-Dade Public Library (1952)

### North Miami

Florida International University North Miami Campus Library (1977)

### Opa Locka

St. Thomas University Library (1977)

### Orlando

University of Central Florida Library (1966)

### Palatka

Saint Johns River Community College Library (1963)

### Panama City

Bay County Public Library (1983)

### Pensacola

University of West Florida John C. Pace Library (1966)

### Port Charlotte

Charlotte County Library System (1973)

### Saint Petersburg

Saint Petersburg Public Library (1965)
Stetson University College of Law Charles A. Dana Library (1975)

### Sarasota

Selby Public Library (1970)

### Tallahassee

Florida Agricultural and Mechanical University Coleman Memorial Library (1936)
Florida State University College of Law Library (1978)
Florida State University Strozier Library (1941)
Florida Supreme Court Library (1974)
State Library of Florida (1929)

### Tampa

Tampa-Hillsborough County Public Library (1965)
University of South Florida Library (1962)
University of Tampa Merl Kelce Library (1953)

### Winter Park

Rollins College Mills Memorial Library (1909)

## GEORGIA

### Albany

Dougherty County Public Library (1964)

### Americus

Georgia Southwestern College James Earl Carter Library (1966)

### Athens

University of Georgia Libraries (1970) REGIONAL
University of Georgia School of Law Library (1979)

### Atlanta

Atlanta-Fulton Public Library (1880)
Atlanta University Center Robert W. Woodruff Library (1962)
Emory University School of Law Library (1968)
Emory University Woodruff Library (1928)
Georgia Institute of Technology Price Gilbert Memorial Library (1963)
Georgia State Library (unknown)
Georgia State University William Russell Pullen Library (1970)
Georgia State University College of Law Library (1983)
U.S. Court of Appeals 11th Circuit Library (1980)

### Augusta

Augusta College Reese Library (1962)

### Brunswick

Brunswick-Glynn County Regional Library (1965)

### Carrollton

West Georgia College Irvine Sullivan Ingram Library (1962)

### Columbus

Columbus College Simon Schwob Memorial Library (1975)

### Dahlonega

North Georgia College Stewart Library (1939)

### Dalton

Dalton Junior College Library Resource Center (1978)

### Macon

Mercer University Stetson Memorial Library (1964)
Mercer University Walter F. George School of Law Library (1978)

### Marietta

Kennesaw College Library (1968)

### Milledgeville

Georgia College at Milledgeville Ina Dillard Russell Library (1950)

### Mount Berry

Berry College Memorial Library (1970)

### Savannah

Chatham-Effingham Liberty Regional Library (1857)

### Statesboro

Georgia Southern College Liberty (1939)

### Valdosta

Valdosta State College Library (1956)

## GUAM

### Agana

Nieves M. Flores Memorial Library (1962)

### Mangilao

University of Guam Robert F. Kennedy Memorial Library (1978)

## HAWAII

### Hilo

University of Hawaii at Hilo Edwin H. Mookini Library (1962)

### Honolulu

Hawaii Medical Library Incorporated (1968)
Hawaii State Library (1929)
Municipal Reference & Records Center (1965)
Supreme Court Law Library (1973)
University of Hawaii Hamilton Library (1907) REGIONAL
University of Hawaii William S. Richardson School of Law Library (1978)

### Laie

Brigham Young University Hawaii Campus, Joseph F. Smith Library (1964)

### Lihue

Kaual Regional Library (1967)

### Pearl City

Leeward Community College Library (1967)

### Wailuku

Maui Public Library (1962)

## IDAHO

### Boise

Boise Public Library and Information Center (1929)
Boise State University Library (1966)
Idaho State Law Library (unknown)
Idaho State Library (1971)

### Cadwell

College of Idaho Terteling Library (1930)

### Moscow

University of Idaho College of Law Library (1978)
University of Idaho Library (1907) REGIONAL

### Nampa

Northwest Nazarene College John E. Riley Library (1984)

### Pocatello

Idaho State University Eli Oboler Library (1908)

### Rexburg

Ricks College Davis O. McKay Learning Resources Center (1946)

### Twin Falls

College of Southern Idaho Library (1970)

## ILLINOIS

### Bloomington

Illinois Wesleyan University Sheean Library (1964)

### Carbondale

Southern Illinois University at Carbondale Morris Library (1932)
Southern Illinois University School of Law Library (1978)

### Carlinville

Blackburn College Lumpkin Library (1954)

### Carterville

Shawnee Library System (1971)

### Champaign

University of Illinois Law Library (1965)

### Charleston

Eastern Illinois University Booth Library (1962)

### Chicago

Chicago Public Library (1876)
Chicago State University Paul and Emily Douglas Library (1954)
DePaul University Law Library (1979)
Field Museum of Natural History Library (1963)
Illinois Institute of Technology Chicago-Kent College of Law Library (1978)
Illinois Institute of Technology Paul V. Galvin Library (1982)
John Marshall Law School Library (1981)
Loyola University of Chicago E. M. Cudahy Memorial Library (1966)
Loyola University School of Law Library (1979)
Northeastern Illinois University Library (1961)
Northwestern University School of Law Library (1978)
University of Chicago Law Library (1964)
University of Chicago Library (1897)
University of Illinois at Chicago Library (1957)
William J. Campbell Library of the U.S. Courts (1979)

### Decatur

Decatur Public Library (1954)

### De Kalb

Northern Illinois University Founders' Memorial Library (1960)
Northern Illinois University College of Law Library (1978)

### Des Plaines

Oakton Community College Library (1976)

### Edwardsville

Southern Illinois University Lovejoy Memorial Library (1959)

### Elsah

Principia College Marshall Brooks Library (1957)

### Evanston

Northwestern University Library (1876)

### Freeport

Freeport Public Library (1905)

### Galesburg

Galesburg Public Library (1896)

### Jacksonville

MacMurray College Henry Pfeiffer Library (1929)

### Kankakee

Olivet Nazarene College Benner Library and Learning Resource Center (1946)

### Lake Forest

Lake Forest College Donnelley Library (1962)

### Lebanon

McKendree College Holman Library (1968)

### Lisle

Illinois Benedictine College Theodore F. Lownik Library (1911)

### Macomb

Western Illinois University Government Publications & Legal Reference Library (1962)

### Moline

Black Hawk College Learning Resources Center (1970)

### Monmouth

Monmouth College Hewes Library (1860)

### Mount Carmel

Wabash Valley College Bauer Media Center (1975)

### Mount Prospect

Mount Prospect Public Library (1977)

### Normal

Illinois State University Milner Library (1877)

### Oak Park

Oak Park Public Library (1963)

### Oglesby

Illinois Valley Community College Jacobs Memorial Library (1976)

### Palos Hills

Moraine Valley Community College Library (1972)

### Peoria

Bradley University Cullom-Davis Library (1963)
Peoria Public Library (1883)

### River Forest

Rosary College Library Rebecca Crown Library (1966)

### Rockford

Rockford Public Library (1895)

### Romeoville

Lewis University Library (1952)

### Springfield

Illinois State Library (unknown) REGIONAL

### Streamwood

Poplar Creek Public Library (1980)

### University Park

Governors' State University Library (1974)

### Urbana

University of Illinois Documents Library (1907)

### Wheaton

Wheaton College Buswell Memorial Library (1964)

### Woodstock

Woodstock Public Library (1963)

## INDIANA

### Anderson

Anderson College Charles E. Wilson Library (1959)
Anderson Public Library (1983)

### Bloomingtron

Indiana University Library (1881)
Indiana University Law Library (1978)

### Crawfordsville

Wabash College Lilly Library (1906)

### Evansville

Evansville and Vanderburgh County Public Library (1928)
Indiana State University at Evansville Evansville Campus Library (1969)

### Fort Wayne

Allen County Public Library (1896)
Indiana University-Purdue University at Fort Wayne Helmke Library (1965)

### Franklin

Franklin College Library (1976)

### Gary

Gary Public Library (1943)
Indiana University Northwest Library (1966)

### Greencastle

De Pauw University Roy O. West Library (1879)

### Hammond

Hammond Public Library (1964)

### Hanover

Hanover College Duggan Library (1892)

### Huntington

Huntington College Loew Alumni Library (1964)

### Indianapolis

Butler University Irwin Library (1965)
Indianapolis-Marion County Public Library (1906)
Indiana State Library (unknown) REGIONAL
Indiana Supreme Court Law Library (1975)
Indiana University School of Law Library (1967)
Indiana University-Purdue University Library (1979)

### Kokomo

Indiana University at Kokmomo Learning Resource Center (1969)

### Muncie

Ball State University Alexander M. Bracken Library (1959)
Muncie Public Library (1906)

### New Albany

Indiana University Southeastern Library (1965)

### Notre Dame

University of Notre Dame Memorial Library (1883)

### Rensselaer

Saint Joseph's College Library (1964)

### Richmond

Earlham College Lilly Library (1964)
Morrison-Reeves Library (1906)

### South Bend

Indiana University at South Bend Library (1965)

### Terre Haute

Indiana State University Cunningham Memorial Library (1906)

### Valparaiso

Valparaiso University Moellering Memorial Library (1930)
Valparaiso University Law Library (1978)

### West Lafayette

Purdue University Libraries (1907)

## IOWA

### Ames

Iowa State University Library (1907)

### Cedar Falls

University of Northern Iowa Library (1946)

### Council Bluffs

Free Public Library (1885)
Iowa Western Community College Herbert Hoover Library (1972)

### Davenport

Davenport Public Library (1973)

### Des Moines

Drake University Cowles Library (1966)
Drake University Law Library (1972)
Public Library of Des Moines (1888)
State Library of Iowa (unknown)

### Dubuque

Carnegie-Stout Public Library (unknown)
Loras College Wahlert Memorial Library (1967)

### Fayette

Upper Iowa University Henderson-Wilder Library (1974)

### Grinnell

Grinnell College Burling Library (1874)

### Iowa City

University of Iowa College of Law Law Library (1968)
University of Iowa Libraries (1884) REGIONAL

### Lamoni

Gracelend College Frederick Madison Smith Library (1927)

### Mason City

North Iowa Area Community College Library (1976)

### Mount Vernon

Cornell College Russell D. Cole Library (1896)

### Orange City

Northwestern College Ramaker Library (1970)

### Sioux City

Sioux City Public Library (1894)

## KANSAS

### Atchison

Benedictine College Library (1965)

### Baldwin City

Baker University Collins Library (1908)

### Colby

Colby Community College H. F. Davis Memorial Library (1968)

### Emporia

Emporia State University William Allen White Library (1909)

### Hays

Fort Hays State University Forsyth Library (1926)

### Hutchinson

Hutchinson Public Library (1963)

### Fort Scott

Fort Scott Community College Learning Resources Center Library (1979)

### Lawrence

University of Kansas Law Library (1971)
University of Kansas Spencer Research Library (1869) REGIONAL

### Manhattan

Kansas State University Farrell Library (1907)

### Pittsburg

Pittsburg State University Leonard H. Axe Library (1952)

### Salina

Kansas Wesleyan University Memorial Library (1930)

### Shawnee Mission

Johnson County Library (1979)

### Topeka

Kansas State Historical Society Library (1877)
Kansas State Library (unknown)
Kansas Supreme Court Law Library (1975)
Washburn University of Topeka Law Library (1971)

### Wichita

Wichita State University Ablah Library (1901)

## KENTUCKY

### Ashland

Boyd County Public Library (1964)

### Barbourville

Union College Abigail E. Weeks Memorial Library (1958)

### Bowling Green

Western Kentucky University Helm-Cravens Library (1934)

### Crestview Hills

Thomas More College Library (1970)

### Danville

Centre College Grace Doherty Library (1884)

### Frankfort

Kentucky Department of Libraries and Archives (1967)
Kentucky State Law Library (unknown)
Kentucky State University Blazer Library (1972)

### Highland Heights

Northern Kentucky University W. Frank Steely Library (1973)

### Lexington

University of Kentucky Law Library (1968)
University of Kentucky Libraries (1907) REGIONAL

### Louisville

Louisville Free Public Library (1904)
University of Louisville Ekstrom Library (1925)
University of Louisville Law Library (1975)

### Morehead

Morehead State University Camden-Carroll Library (1955)

### Murray

Murray State University Waterfield Library (1924)

### Owensboro

Kentucky-Wesleyan College Library Learning Center (1966)

### Richmond

Eastern Kentucky University John Grant Crabbe Library (1966)

### Williamsburg

Cumberland College Norma Perkins Hagan Memorial Library (1983)

## LOUISIANA

### Baton Rouge

Louisiana State Library (1976)
Louisiana State University Middleton Library (1907) REGIONAL
Louisiana State University Paul M. Hebert Law Center Library (1929)
Southern University Law School Library (1979)
Southern University Library (1952)

### Eunice

Louisiana State University at Eunice LeDoux Library (1969)

### Hammond

Southeastern Louisana University Sims Memorial Library (1966)

### Lafayette

University of Southwestern Louisiana Library (1938)

### Lake Charles

McNeese State University Lether E. Frazar Memorial Library (1941)

### Monroe

Northeast Louisiana University Sandel Library (1963)

### Natchitoches

Northwestern State Univewrsity of Louisiana Watson Memorial Library (1887)

### New Orleans

Law Library of Louisiana (unknown)
Loyola University Library (1942)
Loyola University Law Library (1978)
New Orleans Public Library (1883)
Our Lady of Holy Cross College Library (1968)
Southern University in New Orleans Leonard S. Washington Memorial Library (1962)
Tulane University Law Library (1942)
Tulane University Howard-Tilton Memorial Library (1884)
U.S. Court of Appeals Fifth Circuit Library (1973)
University of New Orleans Earl K. Long Library (1963)

### Pineville

Louisiana College Richard W. Norton Memorial Library (1969)

### Ruston

Louisiana Technical University Prescott Memorial Library (1896) REGIONAL

### Shreveport

Louisiana State University at Shreveport Library (1967)
Shreve Memorial Library (1923)

### Thibodaux

Nicholls State University Ellender Memorial Library (1962)

## MAINE

### Augusta

Maine Law and Legislative Reference Library (1973)
Maine State Library (unknown)

### Bangor

Bangor Public Library (1884)

### Brunswick

Bowdoin College Library (1884)

### Castine

Maine Maritime Academy Nutting Memorial Library (1969)

### Lewiston

Bates College George and Helen Ladd Library (1883)

### Orono

University of Maine Raymond H. Fogler Library (1907) REGIONAL

### Portland

Portland Public Library (1884)
University of Maine School of Law Garbrect Law Library (1964)

### Presque Isle

University of Maine at Presque Isle Library Learning Resources Center (1979)

### Sanford

Louis B. Goodall Memorial Library (1984)

### Waterville

Colby College Miller Library (1884)

## MARYLAND

### Annapolis

Maryland State Law Library (unknown)
U.S. Naval Academy Nimitz Library (1895)

### Baltimore

Enoch Pratt Free Library (1887)
Johns Hopkin University Milton S. Eisenhower Library (1882)
Morgan State University Soper Library (1940)
University of Baltimore Langsdale Library (1973)
University of Baltimore Law Library (1980)
University of Maryland School of Law Marshall Law Library (1969)
U.S. Court of Appeals 4th Circuit Library (1982)

### Bel Air

Harford Community College Library (1967)

### Beltsville

Department of Agriculture National Agricultural Library (1895)

### Bethesda

Department of Health and Human Services National Library of Medicine (1978)
Uniformed Services University of Health Sciences Learning Resource Center (1983)

### Catonsville

University of Maryland Baltimore County Albin O. Kuhn Library & Gallery (1971)

### Chestertown

Washington College Clifton M. Miller Library (1891)

### College Park

University of Maryland McKeldin Library (1925) REGIONAL

### Cumberland

Allegany Community College Library (1974)

### Frostburg

Frostburg State College Library (1967)

### Patuxent River

Patuxent River Central Library (1968)

### Rockville

Montgomery County Department of Public Libraries (1951)

### Salisbury

Salisbury State College Blackwell Library (1965)

### Towson

Goucher College Julia Rogers Library (1966)
Towson State University Cook Library (1979)

### Westminster

Western Maryland College Hoover Library (1886)

## MASSACHUSETTS

### Amherst

Amherst College Library (1884)
University of Massachusetts University Library (1907)

### Boston

Boston Athenaeum Library (unknown)
Boston Public Library (1859) REGIONAL
Boston University School of Law Pappas Law Library (1979)
Northeastern University Dodge Library (1962)
State Library of Massachusetts (unknown)
Suffolk University Law Library (1979)
Supreme Judicial Court Social Law Library (1979)
U.S. Court of Appeals First Circuit Library (1978)

### Brookline

Public Library of Brookline (1925)

### Cambridge

Harvard College Library (1860)
Harvard Law School Library (1981)
Massachusetts Institute of Technology Library (1946)

### Chicopee

College of Our Lady of the Elms Alumnae Library (1969)

### Lowell

University of Lowell Alumni-Lydon Library (1952)

### Lynn

Lynn Public Library (1963)

### Medford

Tufts University Wessel Library (1899)

### Milton

Curry College Levin Library (1972)

### New Bedford

New Bedford Free Public Library (1858)

### Newton

Boston College Thomas P. O'Neill Jr. Library (1963)

### Newton Centre

Boston College Law School Library (1979)

### North Dartmouth

Southeastern Massachusetts University Library (1965)

### North Easton

Stonehill College Cushing-Martin Library (1962)

### Springfield

Springfield City Library (1966)
Western New England College Law Library (1978)

### Waltham

Brandeis University Library (1965)
Waltham Public Library (1982)

### Wellesley

Wellesley College Library (1943)

### Wenham

Gordon College Winn Library (1963)

### Williamstown

William College Library (unknown)

### Worcester

American Antiquarian Society Library (1814)
University of Massachusetts Medical Center Lamar Soutter Library (1972)
Worcester Public Library (1859)

## MICHIGAN

### Albion

Albion College Stockwell Memorial Library (1966)

### Allendale

Grand Valley State College Zumberge Library (1963)

### Alma

Alma College Library (1963)

### Ann Arbor

University of Michigan Harlan Hatcher Graduate Library (1884)
University of Michigan Law Library (1978)

### Benton Harbor

Benton Harbor Public Library (1907)

### Bloomfield Hills

Cranbrook Institute of Science Library (1940)

### Dearborn

Henry Ford Centennial Library (1969)
Henry Ford Community College Library (1957)

### Detroit

Detroit College of Law Library (1979)
Detroit Public Library (1868) REGIONAL
Marygrove College Library (1965)
Mercy College of Detroit Library (1965)
University of Detroit Library (1884)
University of Detroit School of Law Library (1978)
Wayne State University G. Flint Purdy Library (1937)
Wayne State University Arthur Neef Law Library (1971)

### Dowagiac

Southwestern Michigan College Matthews Library (1971)

### East Lansing

Michigan State University Documents Library (1907)

### Farmington Hills

Oakland Community College Martin L. King Learning Resources Center (1968)

### Flint

Flint Public Library (1967)
University of Michigan-Flint Library (1977)

### Grand Rapids

Calvin College & Seminary Library (1967)
Grand Rapids Public Library (1876)

### Houghton

Michigan Technological University Library (1876)

### Jackson

Jackson District Library (1965)

### Kalamazoo

Kalamazoo Public Library (1907)
Western Michigan University Dwight B. Waldo Library (1963)

### Lansing

Library of Michigan (unknown) REGIONAL
Thomas M. Cooley Law School Library (1978)

### Livonia

Schoolcraft College Library (1962)

### Madison Heights

Madison Heights Public Library (1982)

### Marquette

Northern Michigan University Olson Library (1963)

### Monroe

Monroe County Library System (1974)

### Mount Clemens

Macomb County Library (1968)

### Mount Pleasant

Central Michigan University Library (1958)

### Muskegon

Hackley Public Library (1894)

### Olivet

Olivet College Library (1974)

### Petoskey

North Central Michigan College Library (1962)

### Port Huron

Saint Clair County Library (1876)

### Rochester

Oakland University Kresge Library (1964)

### Royal Oak

Royal Oak Public Library (1984)

### Saginaw

Hoyt Public Library (1890)

### Sault Ste. Marie

Lake Superior State College Kenneth Shouldice Library (1982)

### Traverse City

Northwestern Michigan College Mark Osterlin Library (1964)

### University Center

Delta College Learning Resources Center (1963)

### Warren

Warren Public Library Arthur J. Miller Branch (1973)

### Wayne

Wayne Oakland Library Federation (1957)

### Ypsilanti

Eastern Michigan University Library (1965)

## MICRONESIA

Community College of Micronesia Library (1982)

## MINNESOTA

### Bemidji

Bemidji State University A.C. Clark Library (1963)

### Blaine

Anoka County Library (1971)

### Collegeville

Saint John's University Alcuin Library (1954)

### Cottage Grove

Washington County Library-Park Grove (1983)

### Duluth

Duluth Public Library (1909)
University of Minnesota Duluth Library (1984)

### Eagan

Dakota County Eagan Library (1983)

### Edina

Southdale-Hennepin Area Library (1971)

### Mankato

Mankato State University Library (1962)

### Minneapolis

Minneapolis Public Library (1893)
University of Minnesota Law School Library (1978)
University of Minnesota Wilson Library (1907) REGIONAL

### Moorhead

Moorhead State University Livingston Lord Library (1956)

### Morris

University of Minnesota, Morris, Rodney A. Briggs Library (1963)

### Northfield

Carleston College Library (1930)
Saint Olaf College Rolvaag Memorial Library (1930)

### Saint Cloud

Saint Cloud State University Learning Rescources Center (1962)

### Saint Paul

Hamline University School of Law Library (1978)
Minnesota Historical Society Library (1867)
Minnesota State Law Library (unknown)
Saint Paul Public Library (1914)
University of Minnesota Saint Paul Campus Library (1974)
William Mitchell College of Law Library (1979)

### Saint Peter

Gustavus Adolphus College Library (1941)

### Willmar

Pioneerland Library (1958)

### Winona

Winona State University Maxwell Library (1969)

## MISSISSIPPI

### Cleveland

Delta State University W. B. Roberts Library (1975)

### Columbus

Mississippi University for Women John Clayton Fant Memorial Library (1929)

### Hattiesburg

University of Southern Mississippi Joseph A. Cook Memorial Library (1935)

### Jackson

Jackson State University Henry Thomas Sampson Library (1968)
Millsaps College Millsaps-Wilson Library (1963)
Mississippi College School of Law Library (1977)
Mississippi Library Commission (1947)
Mississippi State Law Library (unknown)

### Lorman

Alcorn State University Library (1970)

### Mississippi State

Mississippi State University Mitchell Memorial Library (1907)

### Pascagoula

Jackson-George Regional Library (1985)

### University

University of Mississippi J. D. Williams Library (1883) REGIONAL
University of Mississippi James O. Eastland Law Library (1967)

## MISSOURI

### Cape Girardeau

Southeast Missouri State University Kent Library (1916)

### Columbia

University of Missouri at Columbia Library (1862)
University of Missouri-Columbia Law Library (1978)

### Fayette

Central Methodist College George M. Smiley Library (1962)

### Fulton

Westminster College Reeves Library (1875)

### Hillsboro

Jefferson College Library (1984)

### Jefferson City

Lincoln University Inman E. Page Library (1944)
Missouri State Library (1963)
Missouri Supreme Court Library (unknown)

### Joplin

Missouri Southern State College Library (1966)

### Kansas City

Kansas City Missouri Public Library (1881)
Rockhurst College Greenlease Library (1917)
University of Missouri at Kansas City General Library (1938)
University of Missouri-Kansas City Leon E. Bloch Law Library (1978)

### Kirksville

Northeast Missouri State University Pickler Memorial Library (1966)

### Liberty

William Jewell College Charles F. Curry Library (1900)

### Maryville

Northwest Missouri State University B. D. Owens Library (1982)

### Rolla

University of Missouri-Rolla Curtis Laws Wilson Library (1907)

### Saint Charles

Lindenwood College Margaret Leggat Butler Library (1973)

### Saint Joseph

Saint Joseph Public Library (1891)

### Saint Louis

Marysville College Library (1976)
Saint Louis County Library (1970)
Saint Louis Public Libary (1866)
Saint Louis University Law Library (1967)
Saint Louis University Pius XII Memorial Library (1866)
U.S. Court of Appeals Eighth Circuit Library (1972)
University of Missouri at Saint Louis Thomas Jefferson Library (1966)
Washington University John M. Olin Library (1906)
Washington University Law Library (1978)

### Springfield

Drury College, Walker Library (1874)
Southwest Missouri State University Library (1963)

### Warrensburg

Central Missouri State University Ward Edwards Library (1914)

## MONTANA

### Billings

Eastern Montana College Library (1958)

### Bozeman

Montana State University Renne Library (1907)

### Butte

Montana College of Mineral Science and Technology Library (1901)

### Havre

Northern Montana College Vande Bogart Library (1980)

### Helena

Carroll College Library (1974)
Montana State Library (1966)
State Law Library of Montana (1977)

### Missoula

University of Montana Maurene & Mike Mansfield Library (1909) REGIONAL

## NEBRASKA

### Blair

Dana College Dana-LIFE Library (1924)

### Crete

Doane College Perkins Library (1944)

### Fremont

Midland Lutheran College Luther Library (1924)

### Kearney

Kearney State College Calvin T. Ryan Library (1962)

### Lincoln

Nebraska Library Commission (1972)
Nebraska State Library (unknown)
University of Nebraska-Lincoln College of Law Library (1981)
University of Nebraska-Lincoln D. L. Love Memorial Library (1907) REGIONAL

### Omaha

Creighton University Reinert/Alumni Library (1964)
Creighton University School of Law Library (1979)
Omaha Public Library W. Dale Clark Library (1980)
University of Nebraska at Omaha University Library (1939)

### Scottsbluff

Scottsbluff Public Library (1925)

### Wayne

Wayne State College U.S. Conn Library (1970)

## NEVADA

### Carson City

Nevada State Library (unknown)
Nevada Supreme Court Library (1973)

### Las Vegas

Las Vegas-Clark County Library (1974)
University of Nevada at Las Vegas James Dickinson Library (1959)

### Reno

National Judicial College Law Library (1979)
Nevada Historical Society Library (1974)
University of Nevada-Reno Library (1907) REGIONAL
Washoe County Library (1980)

## NEW HAMPSHIRE

### Concord

Franklin Pierce Law Center Library (1973)
New Hampshire State Library (unknown)

### Durham

University of New Hampshire Library (1907)

### Hanover

Dartmouth College Library (1884)

### Henniker

New England College Danforth Library (1966)

### Manchester

Manchester City Library (1884)
New Hampshire College H. A. B. Shapiro Memorial Library (1976)
Saint Anselm College Geisel Library (1963)

### Nashua

Nashua Public Library (1971)

## NEW JERSEY

### Bayonne

Bayonne Free Public Library (1909)

### Bloomfield

Bloomfield Public Library (1965)

### Bridgeton

Cumberland County Library (1966)

### Camden

Rutgers University Camden Library (1966)
Rutgers University School of Law Library (1979)

### Convent Station

College of Saint Elizabeth Mahoney Library (1938)

### East Brunswick

East Brunswick Public Library (1977)

### East Orange

East Orange Public Library (1966)

### Elizabeth

Free Public Library of Elizabeth (1895)

### Glassboro

Glassboro State College Savitz Learning Resource Center (1963)

### Hackensack

Johnson Free Public Library (1966)

### Irvington

Irvington Public Library (1966)

### Jersey City

Jersey City Public Library (1879)
Jersey City State College Forest A. Irwin Library (1963)

### Lawrenceville

Rider College Franklin F. Moore Library (1975)

### Madison

Drew University Library (1939)

### Mahwah

Ramapo College Library (1971)

### Mount Holly

Burlington County Library (1966)

### New Brunswick

New Brunswick Free Public Library (1908)
Rutgers University Alexander Library (1907)

### Newark

Newark Public Library (1906) REGIONAL
Rutgers-The State University of New Jersey John Cotton Dana Library (1966)
Rutgers University Law School, Ackerson Law Library (1979)
Seton Hall University Law Library (1979)

### Passaic

Passaic Public Library (1964)

### Pemberton

Burlington County College Library (1979)

### Phillipsburg

Phillipsburg Free Public Library (1976)

### Plainfield

Plainfield Public Library (1971)

### Pomona

Stockton State College Library (1972)

### Princeton

Princeton University Library (1884)

### Randolph

County College of Morris Sherman H. Masten Learning Resource Center (1975)

### Rutherford

Fairleigh Dickinson University Messler Library (1953)

### Shrewsbury

Monmouth County Library (1968)

### South Orange

Seton Hall University McLaughlin Library (1947)

### Teaneck

Fairleigh Dickinson University Teaneck/Hackensack Campus Weiner Library (1963)

### Toms River

Ocean County College Learning Resources Center (1966)

### Trenton

New Jersey State Library (unknown)
Trenton Free Public Library (1902)

### Union

Kean College of New Jersey Nancy Thompson Library (1971)

### Upper Montclair

Montclair State College Harry A. Sprague Library (1967)

### Wayne

Wayne Public Library (1972)

### West Long Branch

Monmouth College Guggenheim Memorial Library (1963)

### Woodbridge

Woodbridge Public Library (1965)

## NEW MEXICO

### Albuquerque

University of New Mexico Medical Center Library (1973)
University of New Mexico School of Law Library (1973)
University of New Mexico General Library (1896) REGIONAL

### Hobbs

New Mexico Junior College Pannell Library (1969)

### Las Cruces

New Mexico State University Library (1907)

### Las Vegas

New Mexico Highlands University Donnelly Library (1913)

### Portales

Eastern New Mexico University Golden Library (1962)

### Santa Fe

New Mexico State Library (1960) REGIONAL
New Mexico Supreme Court Law Library (unknown)

### Silver City

Western New Mexico University Miller Library (1972)

### Socorro

New Mexico Institute of Mining & Technology Martin Speare Memorial Library (1984)

## NEW YORK

### Albany

Albany Law School Library (1979)
New York State Library (unknown ) REGIONAL
State University of New York at Albany University Library (1964)

### Auburn

Seymour Library (1972)

### Bayside

CUNY Law School at Queens College CUNY Law Library (1983)

### Binghamton

State University New York at Binghamton Glenn G. Bartle Library (1962)

### Brockport

State University of New York at Brockport Drake Memorial Library (1967)

### Bronx

Fordham University Library (1937)
Herbert H. Lehman College Library (1967)
New York Public Library (1973)
State University of New York Maritime College Stephen B. Luce Library (1947)

### Bronxville

Sarah Lawrence College Esther Raushensh Library (1910)

### Brooklyn

Brooklyn College Library (1936)
Brooklyn Law School Library (1974)
Brooklyn Public Library (1908)
Brooklyn Public Library Business Library (1984)
Pratt Institute Library (1891)
State University of New York Downstate Medical Center Library (1958)

### Buffalo

Buffalo and Erie County Public Library (1895)
State University of New York at Buffalo Charles B. Sears Law Library (1978)
State University of New York at Buffalo Lockwood Memorial Library (1963)

### Canton

Saint Lawrence University Owen D. Young Library (1920)

### Corning

Corning Community College Arthur A. Houghton Jr. Library (1963)

### Cortland

State University of New York College at Cortland Memorial Library (1964)

### Delhi

State University Agricultural and Technical College Library (1970)

### Douglaston

Cathedral College Library (1971)

### East Islip

East Islip Public Library (1973)

### Elmira

Elmira College Gannett Tripp Learning Center (1956)

### Farmingdale

State University of New York at Farmingdale Greenley Library (1917)

### Flushing

Queens College Paul Klapper Library (1939)

### Garden City

Adelphi University Swirbul Library (1966)

### Geneseo

State University of New York at Geneseo Milne Library (1967)

### Greenvale

Long Island University B. Davis Schwartz Memorial Library (1964)

### Hamilton

Colgate University, Everett Needham Case Library (1902)

### Hempstead

Hofstra University Library (1964)
Hofstra University School of Law Library (1979)

### Huntington

Touro College School of Law Library (1985)

### Ithaca

Cornell University Library (1907)
Cornell Law Library (1978)
New York State College of Agriculture and Human Ecology Albert R. Mann Library (1943)

### Jamaica

Queens Borough Public Library (1926)
Saint John's University Library (1956)
Saint John's University School of Law Library (1978)

### Kings Point

U.S. Merchant Marine Academy Schuyler Otis Bland Library (1962)

### Long Island City

Fiorello H. LaGuardia Community College Library (1981)

### Mount Vernon

Mount Vernon Public Library (1962)

### New Paltz

State University College at New Paltz Sojourner Truth Library (1965)

### New York City

City College of City University of New York Library (1884)
College of Insurance Library (1965)
Columbia University Libraries (1882)
Columbia University School of Law Library (1981)
Cooper Union for the Advancement of Science and Arts Library (1930)
Medical Library Center of New York (1976)
New York Law Institute Library (1909)
New York Law School Library (1979)
New York Public Library (1907)
New York Public Library (1884)
New Yrok University Law Library (1974)
New York University Elmer Holmes Bobst Library (1967)
U.S. Court of Appeals Second Circuit Library (1976)
Yeshiva University Chutick Law Library Cordoza School of Law (1979)
Yeshiva University Pollack Library (1979)

### Newburgh

Newburgh Free Library (1909)

### Niagara Falls

Niagara Falls Public Library (1976)

### Oakdale

Dowling College Library (1965)

### Oneonta

State University College at Onenonta James M. Miline Library (1966)

### Oswego

State University of New York at Oswego Penfield Library (1966)

### Plattsburgh

State University College at Plattsburgh Benjamin F. Feinberg Library (1967)

### Potsdam

Clarkson University Harriet Call Burnap Memorial Library (1938)
State University College at Potsdam Frederick W. Crumb Memorial Library (1964)

### Poughkeepsie

Vassar College Library (1943)

### Purchase

State University of New York, College of Purchase Library (1969)

### Rochester

Rochester Public Library (1963)
University of Rochester Rush Rhees Library (1880)

### Saint Bonaventure

Saint Bonaventure University Friedsam Memorial Library (1938)

### Saratoga Springs

Skidmore College Library (1964)

### Schenectady

Union College Schaffer Library (1901)

### Southampton

Long Island University Southhampton Campus Library (1973)

### Sparkill

St. Thomas Aquinas College Lougheed Library (1984)

### Staten Island

Wagner College Horrmann Library (1953)

### Stony Brook

State University of New York at Stony Brook Main Library (1963)

### Syracuse

Onondaga County Public Library (1978)
Syracuse University Bird Library (1878)
Syracuse University College of Law H. Doughlas Barclay Law Library (1978)

### Troy

Troy Public Library (1869)

### Uniondale

Nassau Library System (1965)

### Utica

Utica Public Library (1885)
SUNY College of Technology Library (1977)

### West Point

U.S. Millitary Academy Library (unknown)

### White Plains

Pace University Law School Library (1978)

### Yonkers

Yonkers Public Library Getty Square Branch (1910)

### Yorktown Heights

Mercy College Library (1976)

## NORTH CAROLINA

### Asheville

University of North Carolina at Asheville D. Hiden Ramsey Library (1965)

### Boiling Springs

Gardner-Webb College Dover Memorial Library (1974)

### Boone

Appalachian State University Carol Grotnes Belk Library (1963)

### Buies Creek

Campbell University Carrie Rich Memorial Library (1965)

### Chapel Hill

University of North Carolina at Chapel Hill Davis Library (1884) REGIONAL
University of North Carolina Law Library (1978)

### Charlotte

Public Library of Charlotte and Mecklenburg County (1964)
Queens College Everett Library (1927)
University of North Carolina at Charlotte Atkins Library (1964)

### Cullowhee

Western Carolina University Hunter Library (1953)

### Davidson

Davidson College Library (1893)

### Durham

Duke University School of Law Library (1978)
Duke University William R. Perkins Library (1890)
North Carolina Central University Law Library (1979)
North Carolina Central University James E. Shepard Memorial Library (1973)

### Elon College

Elon College Iris Holt McEwen Library (1971)

### Fayetteville

Fayetteville State University Charles W. Chesnutt Library (1971)

### Greensboro

North Carolina Agricultural and Technical State University F. D. Bluford Library (1937)
University of North Carolina at Greensboro Walter Clinton Jackson Library (1963)

### Greenville

East Carolina University J. Y. Joyner Library (1951)

### Laurinburg

Saint Andrews Presbyterian College DeTamble Library (1969)

### Lexington

Davidson County Public Library (1971)

### Mount Olive

Mount Olive College Moye Library (1971)

### Murfreesboro

Chowan College Whitaker Library (1963)

### Pembroke

Pembroke State University Mary H. Livermore Library (1956)

### Raleigh

Department of Cultural Resources Division of State Library (unknown)
North Carolina State University D. H. Hill Library (1923)
North Carolina Supreme Court Library (1972)

### Rocky Mount

North Carolina Wesleyan College Library (1969)

### Salisbury

Catawba College Library (1925)

### Wilmington

University of North Carolina at Wilmington William M. Randall Library (1965)

### Wilson

Atlantic Cristian College Hackney Library (1930)

### Winston-Salem

Forsyth County Public Library (1954)
Wake Forest University Z. Smith Reynolds Library (1902)

## NORTH DAKOTA

### Bismarck

North Dakota State Library (1971)
North Dakota Supreme Court Law Library (unknown)
State Historical Society of North Dakota State Archives & Historical Research Library (1907)
Veteran's Memorial Public Library (1967)

### Dickinson

Dickinson State College Stoxen Library (1968)

### Fargo

Fargo Public Library (1964)
North Dakota State University Library (1907) REGIONAL

### Grand Forks

University of North Dakota Chester Fritz Library (1890)

### Minot

Minot State College Memorial Library (1925)

### Valley City

Valley City State College Library (1913)

## OHIO

### Ada

Ohio Northern University J. P. Taggart Law Library (1965)

### Akron

Akron-Summit County Public Library (1952)
University of Akron Bierce Library (1963)
University of Akron School of Law Library (1978)

### Alliance

Mount Union College Library (1888)

### Ashland

Ashland College Library (1938)

### Athens

Ohio University Alden Library (1886)

### Batavia

University of Cincinnati at Batavia Clermont General and Technical College Library (1973)

### Bluffton

Bluffton College, Musselman Library (1951)

### Bowling Green

Bowling Green State University Jerome Library (1933)

### Canton

Malone College Everett L. Cattell Library (1970)

### Chardon

Geauga County Public Library (1971)

### Cincinnati

Public Library of Cincinnati and Hamilton County (1884)
University of Cincinnati Central Library (1929)
University of Cincinnati College of Law (1978)

### Cleveland

Case Western Reserve University Freiberger Library (1913)
Case Western Reserve University School of Law Library (1979)
Cleveland Public Library (1886)
Cleveland State University Cleveland-Marshall College of Law Joseph W. Bartunek III Law Library (1978)
Cleveland State University Library (1966)
Municipal Reference Library (1970)

### Cleveland

Cleveland Heights-University Heights Public Library (1970)

### Columbus

Capital University Law School Library (1980)
Capital University Library (1968)
Ohio State University College of Law Library (1984)
Ohio State University Libraries (1907)
Ohio Supreme Court Law Library (1973)
Public Library of Columbus and Franklin County (1885)
State Library of Ohio (unknown) REGIONAL

### Dayton

Dayton and Montgomery County Public Library (1909)
University of Dayton Roesch Library (1969)
Wright State University Library (1965)

### Delaware

Ohio Wesleyan University L. A. Beeghly Library (1845)

### Elyria

Elyria Public Library (1966)

### Findlay

Findlay College Shafer Library (1969)

### Gambier

Kenyon College Library (1873)

### Granville

Denison University Libraries William H. Doane Library (1884)

### Hiram

Hiram College Teachout-Price Memorial Library (1874)

### Kent

Kent State University Libraries (1962)

### Marietta

Marietta College Dawes Memorial Library (1884)

### Marion

Marion Public Library (1979)

### Middletown

Miami University-Middletown Gardner-Harvey Library (1970)

### New Concord

Muskingum College Library (1966)

### Oberlin

Oberlin College Library (1858)

### Oxford

Miami University Library King Library (1909)

### Portsmouth

Portsmouth Public Library (unknown)

### Rio Grande

Rio Grande College and Community College Jeanette Albiez Davis Library (1966)

### Springfield

Warder Public Library (1884)

### Steubenville

University of Steubenville Starvaggi Memorial Library (1971)
Public Library of Steubenville and Jefferson County (1950)

### Tiffin

Heidelberg College Beeghly Library (1964)

### Toledo

Toledo-Lucus County Public Library (1884)
University of Toledo College of Law Library (1981)
University of Toledo Library (1963)

### University Heights

John Carroll University Grasselli Library (1963)

### Westerville

Otterbein College Courtright Memorial Library (1967)

### Wooster

College of Wooster Andrews Library (1966)

### Worthington

Worthington Public Library (1984)

### Youngstown

Public Library of Youngstown and Mahoning County (1923)
Youngstown State University William F. Maag Library (1971)

## OKLAHOMA

### Ada

East Central Oklahoma State University Linscheid fLibrary (1914)

### Alva

Northwestern Oklahoma State University J. W. Martin Library (1907)

### Bethany

Bethany Nazarene College R. T. Williams Learning Resources Center (1971)

### Durant

Southeastern Oklahoma State University Henry G. Bennett Memorial Library (1929)

### Edmond

Central State University Library (1934)

### Enid

Public Library of Enid and Garfield County (1908)

### Langston

Langston University G. Lamar Harrison Library (1941)

### Muskogee

Muskogee Public Library (1971)

### Norman

University of Oklahoma Libraries Bizzell Memorial Library (1893)
University of Oklahoma Law Library (1978)

### Oklahoma City

Metropolitan Library System Main Library (1974)
Oklahoma City University Dulaney Browne Library (1963)
Oklahoma Department of Libraries (1893) REGIONAL

### Shawnee

Oklahoma Baptist University Library (1933)

### Stillwater

Oklahoma State University Library (1907) REGIONAL

### Tahlequah

Northeastern Oklahoma State University John Vaughan Library (1923)

### Tulsa

Tulsa City-County Library System (1963)
University of Tulsa College of Law Library (1979)
University of Tulsa McFarlin Library (1929)

### Weatherford

Southwestern Oklahoma State University Al Harris Library (1958)

## OREGON

### Ashland

Southern Oregon State College Library (1953)

### Corvallis

Oregon State University Library (1907)

### Eugene

University of Oregon Law Library (1979)
University of Oregon Library (1883)

### Forest Grove

Pacific University Harvey W. Scott Memorial Library (1897)

### Klamath Falls

Oregon Institute of Technology Library (1982)

### La Grande

Eastern Oregon State College Walter M. Pierce Library (1954)

### McMinnville

Linfield College Northup Library (1965)

### Monmouth

Western Oregon State College Library (1967)

### Pendleton

Blue Mountain Community College Library (1983)

### Portland

Lewis and Clark College Aubrey R. Watzek Library (1967)
Library Association of Portland (1884)
Northwestern School of Law Lewis and Clark College Paul L. Boley Law Library (1979)
Portland State University Millar Library (1963) REGIONAL
Reed College Library (1912)
U.S Department of Engery Bonneville Power Administration Library (1962)

### Salem

Oregon State Library (unknown)
Oregon Supreme Court Law Library (1974)
Williamette University College of Law Library (1979)
Williamette University Main Library (1969)

## PENNSYLVANIA

### Allentown

Muhlenberg College Haas Library (1939)

### Altoona

Altoona Area Public Library (1969)

### Bethel Park

Bethel Park Public Library (1980)

### Bethlehem

Lehigh University Libraries Liderman Library (1876)

### Blue Bell

Montgomery County Community College Learning Resources Center (1975)

### Bradford

University of Pittsburgh at Bradford Bradford Campus Library (1979)

### Carlisle

Dickinson College Boyd Lee Spahr Library (1947)
Dickinson School of Law Sheeley-Lee Law Library (1978)

### Cheyney

Cheyney University Leslie Pinckney Hill Library (1967)

### Collegeville

Ursinus College Myrin Library (1963)

### Coraopolis

Robert Morris Coillege Library (1978)

### Doylestown

Bucks County Free Library (1970)

### East Stroudsburg

East Stroudsburg University Kemp Library (1966)

### Erie

Erie County Library System (1897)

### Greenville

Thiel College Langenheim Memorial Library (1963)

### Harrisburg

State Library of Pennsylvania (unknown) REGIONAL

### Haverford

Haverford College Magill Library (1897)

### Hazleton

Hazleton Area Public Library (1964)

### Indiana

Indiana University of Pennsylvania Rodes R. Stabley Library (1962)

### Johnstown

Cambria County Library System Glosser Memorial Library Building (1965)

### Lancaster

Franklin and Marshall College Shadek-Fackenthal Library (1895)

### Lewisburg

Bucknell University Ellen Clarke Bertrand Library (1963)

### Mansfield

Mansfield University Library (1968)

### Meadville

Allegheny College Lawrence Lee Pelletier Library (1907)

### Millersville

Millersville University Helen A. Ganser Library (1966)

### Monessen

Monessen Public Library (1969)

### New Castle

New Castle Public Library (1963)

### Newtown

Bucks County Community College Library (1968)

### Norristown

Montgomery County Norristown Public Library (1969)

### Philadelphia

Drexel University Library (1963)
Free Library of Philadelphia (1897)
Saint Joseph's University Drexel Library (1974)
Temple University Paley Library (1947)
Temple University Law Library (1979)
Thomas Jefferson University Scott Memorial Library (1978)
U.S. Court of Appeals Third Circuit Library (1973)
University of Pennsylvania Biddle Law Library (1974)
University of Pennsylvania Library (1886)

### Pittsburgh

Allegheny County Law Library (1977)
Carnegie Library of Pittsburgh (1895)
Carnegie Library of Pittsburgh Allegheny Regional Branch (1924)
Duquesne University Law Library (1978)
La Roche College John J. Wright Library (1974)
U.S. Department of Interior Bureau of Mines Library (1962)
University of Pittsburgh Hillman Library (1910)
University of Pittsburgh Law Library (1979)

### Pottsville

Pottsville Free Public Library (1967)

### Reading

Reading Public Library (1901)

### Scranton

Scranton Public Library (1895)

### Shippensburg

Shippensburg University Ezra Lehman Memorial Library (1973)

### Slippery Rock

Slippery Rock University Bailey Library (1965)

### Swarthmore

Swarthmore College McCabe Library (1923)

### University Park

Pennsylvania State University Libraries Pattee Library (1907)

### Villanova

Villanova University Law School Pulling Law Library (1964)

### Warren

Warren Library Association Warren Public Library (1885)

### Washington

Washington and Jefferson College U. Grant Miller Library (1884)

### Waynesburg

Waynesburg College Library (1964)

### West Chester

West Chester University Francis Harvey Green Library (1967)

### Wilkes-Barre

King's College D. Leonard Corgan Library (1949)

### Williamsport

Lycoming College Library (1970)

### York

York College of Pennsylvania Schmidt Library (1963)

### Youngwood

Westmoreland County Community College Learning Resources Center (1972)

## PUERTO RICO

### Mayaguez

University of Puerto Rico Mayaguez Campus Library (1928)

### Ponce

Catholic University of Puerto Rico Encarnacion Valdes Library (1966)
Catholic University of Puerto Rico School of Law Library (1978)

### Rio Piedras

University of Puerto Rico J. M. Lazaro Library (1928)

## RHODE ISLAND

### Kingston

University of Rhode Island Library (1907)

### Newport

U.S. Naval War College Library (1963)

### Providence

Brown University John D. Rockefeller Jr. Library (unknown)
Providence College Phillips Memorial Library (1969)
Providence Public Library (1884)
Rhode Island College James P. Adams Library (1965)
Rhode Island State Law Library (1979)
Rhode Island State Library (1895)

### Warwick

Warwick Public Library (1966)

### Westerly

Westerly Public Library (1909)

### Woonsocket

Woonsocket Harris Public Library (1977)

## SOUTH CAROLINA

### Charleston

Baptist College at Charleston L. Mendel Rivers Library (1967)
The Citadel Millitary College Daniel Library (1962)
College of Charleston Robert Scott Small Library (1869)

### Clemson

Clemson University Cooper Library (1893)

### Columbia

Benedict College Payton Learning Resources Center (1969)
South Carolina State Library (1895)
University of South Carolina Coleman Karesh Law Library (1983)
University of South Carolina Thomas Cooper Library (1884)

### Conway

University of South Carolina Coastal Carolina College Kimbel Library (1974)

### Due West

Erskine College McCain Library (1968)

### Florence

Florence County Library (1967)
Francis Marion College James A. Rogers Library (1970)

### Greenville

Furman University Library (1962)
Greenville County Library (1966)

### Greenwood

Lander College Larry A. Jackson Library (1967)

### Orangeburg

South Carolina State College Miller F. Whittaker Library (1953)

### Rock Hill

Winthrop College Dacus Library (1896)

### Spartansburg

Spartansburg County Public Library (1967)

## SOUTH DAKOTA

### Aberdeen

Northern State College Beulah Williams Library (1963)

### Brookings

South Dakota State University H. M. Briggs Library (1889)

### Pierre

South Dakota State Library (1973)
South Dakota Supreme Court Library (1978)

### Rapid City

Rapid City Public Library (1963)
South Dakota School of Mines and Technology Devereaux Library (1963)

### Sioux Falls

Augustana College Mikkelsen Library (1969)
Sioux Falls Public Library (1903)

### Spearfish

Black Hills State College Library Learning Center (1942)

### Vermillion

University of South Dakota I. D. Weeks Library (1889)

## TENNESSEE

### Bristol

King College E. W. King Library (1970)

### Chattanooga

Chattanooga-Hamilton County Bicentennial Library (1908)
U.S. Tennessee Valley Authority Technical Library (1976)

### Clarksville

Austin Peay State University Felix G. Woodward Library (1945)

### Cleveland

Cleveland State Community College Library (1973)

### Columbia

Columbia State Community College John W. Finney Memorial Library (1973)

### Cookeville

Tennessee Technological University Jere Whitson Memorial Library (1969)

### Jackson

Lambuth College Luther L. Gobbel Library (1967)

### Jefferson City

Carson-Newman College Library (1964)

### Johnson City

East Tennessee State University Sherrod Library (1942)

### Knoxville

Knoxville County Public Library System Lawson McGhee Library (1973)
University of Tennessee at Knoxville James D. Hoskins Library (1907)
University of Tennessee Law Library (1971)

### Martin

University of Tennessee at Martin Paul Meek Library (1957)

### Memphis

Mamphis-Shelby County Public Library and Information Center (1896)
Memphis State University Cecil C. Humphreys School of Law Library (1979)
Memphis State University Libraries (1966)

### Murfreesboro

Middle Tennessee State University Todd Library (1912)

### Nashville

Fisk University Library (1965)
Public Library of Nashville and Davidson County (1884)
Tennessee State Law Library (1976)
Tennessee State Library and Archives (unknown)
Tennessee State University Brown-Daniel Library (1972)
Vanderbilt University Alyne Queener Massey Law Library (1976)
Vanderbilt University Library (1884)

### Sewanee

University of the South Jessie Ball duPont Library (1873)

## TEXAS

### Abilene

Abilene Christian University Margaret and Herman Brown Library (1978)
Hardin-Simmons University Rupert and Pauline Richardson Library (1940)

### Arlington

Arlington Public Library (1970)
University of Texas at Arlington Library (1963)

### Austin

Texas State Law Library (1972)
Texas State Library (unknown) REGIONAL
University of Texas at Austin Perry-Castañeda Library (1884)
University of Texas at Austin Edie and Lew Wasserman Public Affairs Library (1966)
University of Texas at Austin Tarlton Law Library (1965)

### Baytown

Lee College Library (1970)

### Beaumont

Lamar University Mary and John Gray Library (1957)

### Brownwood

Howard Payne University Walker Memorial Library (1964)

### Canyon

West Texas State University Cornette Library (1928)

### College Station

Texas Agricultural and Mechanical University David G. Evans Library (1907)

### Commerce

East Texas State University James Gilliam Gee Library (1937)

### Corpus Christi

Corpus Christi State University Library (1976)

### Corsicana

Navarro College Gaston T. Gooch Library (1965)

### Dallas

Bishop College Zale Library (1966)
Dallas Baptist University Vance Memorial Library (1967)
Dallas Public Library (1900)
Southern Methodist University Fondren Library (1925)
University of Texas Health Science Center-Dallas Library (1975)

### Denton

North Texas State University Library (1948)

### Edinburg

Pan American University Library (1959)

### El Paso

El Paso Public Library (1906)
University of Texas at El Paso Library Documents & Maps Library (1966)

### Fort Worth

Fort Worth Public Library (1905)
Texas Christian University Mary Couts Burnett Library (1916)

### Galveston

Rosenberg Library (1909)

### Houston

Houston Public Library (1884)
North Harris County College Learning Resource Center (1974)
Rice University Fondren Library (1967)
South Texas College of Law Library (1981)
Texas Southern University Thurgood Marshall School of Law Library (1982)
University of Houston-Clear Lake Alfred R. Neumann Library (1980)
University of Houston Library (1957)
University of Houston School of Law Librray (1979)

### Huntsville

Sam Houston State University Newton Gresham Library (1949)

### Irving

Irving Public Library System (1974)

### Kingsville

Texas Arts and Industries University Jernigan Library (1944)

### Laredo

Laredo Junior College Harold R. Yeary Library (1970)

### Longview

Nicholson Memorial Public Library (1961)

### Lubbock

Texas Tech University Library (1935) REGIONAL
Texas Tech University School of Law Library (1978)

### Marshall

Wiley College Thomas Winston Cole Sr. Library (1962)

### Nacogdoches

Stephen F. Austin State University Steen Library (1965)

### Plainview

Wayland Baptist University Van Howeling Memorial Library (1963)

### Richardson

University of Texas at Dallas McDermott Library (1972)

### San Angelo

Angelo State University Port Henderson Library (1964)

### San Antonia

Saint Mary's University Academic Library (1964)
Saint Mary's University Law Library (1982)
San Antonio College Library (1972)
San Antonio Public Library (1899)
Trinity University Elizabeth Coates Maddux Library (1964)
University of Texas at San Antonio Library (1973)

### San Marcos

Southwest Texas State University Library (1955)

### Seguin

Texas Lutheran College Blumberg Memorial Library (1970)

### Sherman

Austin College Arthur Hopkins Library (1963)

### Texarkana

Texarkana Community College Palmer Memorial Library (1963)

### Victoria

Victoria College/University of Houston Victoria Campus Library (1973)

### Waco

Baylor University Law Library (1982)
Baylor University Moody Memorial Library (1905)

### Wichita Falls

Midwestern State University Moffett Library (1963)

## UTAH

### Cedar City

Southern Utah State College Library (1964)

### Ephraim

Snow College Lucy A. Phillips Library (1963)

### Logan

Utah State University Merrill Library and Learning Resources Center (1907) REGIONAL

### Ogden

Weber State College Stewart Library (1962)

### Provo

Brigham Young University Harold B. Lee Library (1908)
Brigham Young University Law Library (1972)

### Salt Lake City

University of Utah Eccles Health Sciences Library (1970)
University of Utah Law Library (1966)
University of Utah Marriott Library (1893)
Utah State Library (unknown)
Utah State Supreme Court Law Library (1975)

## VERMONT

### Burlington

University of Vermont Bailey/Howe Library (1907)

### Castleton

Castleton State College Calvin Coolidge Library (1969)

### Johnson

Johnson State College John Dewey Library (1955)

### Lyndonville

Lyndon State College Samuel Reed Hall Library (1969)

### Middlebury

Middlebury College Egbert Starr Library (1884)

### Montpelier

Vermont Department of Libraries (1845)

### Northfield

Norwich University Library (1908)

### South Royalton

Vermont Law School Library (1978)

## VIRGIN ISLANDS

### Saint Croix

Florence Williams Public Library (1968)

### Saint Thomas

College of the Virgin Islands Ralph M. Paiewonsky Library (1973)
Enid M. Baa Library and Archives (1968)

## VIRGINA

### Alexandria

Dept. of the Navy Office of Judge Advocate General Law Library (1963)

### Arlington

George Mason University School of Law Library (1981)

### Blacksburg

Virginia Polytechnic Institute and State University Carol M. Newman Library (1907)

### Bridgewater

Bridgewater College Alexander Mack Memorial Library (1902)

### Charlottesville

University of Virginia Alderman Library (1910) REGIONAL
University of Virginia Arthur J. Morris Law Library (1964)

### Chesapeake

Chesapeake Public Library (1970)

### Danville

Danville Community College Learning Resources Center (1969)

### Emory

Emory and Henry College Kelly Library (1884)

### Fairfax

George Mason University Fenwick Library (1960)

### Fredericksburg

Mary Washington College E. Lee Trinkle Library (1940)

### Hampden-Sydney

Hampden-Sydney College Eggleston Library (1891)

### Hampton

Hampton Institute Huntington Memorial Library (1977)

### Harrisonburg

James Madison University Carrier Library (1973)

### Hollins College

Hollins College Fishburn Library (1967)

### Lexington

Virginia Military Institute Preston Library (1874)
Washington and Lee University University Library (1910)
Washington and Lee University Wilbur C. Hall Law Library (1978)

### Martinsville

Patrick Henry Community College Library (1971)

### Norfolk

Norfolk Public Library (1895)
Old Dominion University Library (1963)
U.S. Armed Forces Staff College Library (1963)

### Petersburg

Virginia State University Johnston Memorial Library (1907)

### Quantico

Federal Bureau of Investigation Academy Library (1970)
Marine Corps Education Center MCDEC James Carson Breckinridge Library (1967)

### Reston

Department of the Interior Geological Survey Library (1963)

### Richmond

U.S. Court of Appeals Fourth Circuit Library (1973)
University of Richmond Boatwright Memorial Library (1900)
University of Richmond Law School Library (1982)
Virginia Commonwealth University James Branch Cabell Library (1971)
Virginia State Law Library (1973)
Virginia State Library (unknown)

### Salem

Roanoke College Library (1886)

### Williamsburg

College of William and Mary Marshall-Wythe Law Library (1978)
College of William and Mary Swem Library (1936)

### Wise

Clinch Valley College John Cook Wyllie Library (1971)

## WASHINGTON

### Bellingham

Western Washington University Mable Zoe Wilson Library (1963)

### Cheney

Eastern Washington University JFK Library (1966)

### Ellensburg

Central Washington University Library (1962)

### Everett

Everett Public Library (1914)

### Midway

Highline Community College Library (1983)

### Olympia

Evergreen State College Daniel J. Evans Library (1972)
Washington State Law Library (1979)
Washington State Library (unknown) REGIONAL

### Port Angeles

North Olympic Library System (1965)

### Pullman

Washington State University Holland Library

### Seattle

Seattle Public Library (1908)
University of Washington Suzallo Library (1890)
University of Washington Marian Gould Gallagher Law Library (1969)
U.S. Court of Appeals 9th Circuit Library (1981)

### Spokane

Gonzaga University School of Law Library (1979)
Spokane Public Library (1910)

### Tacoma

Tacoma Public Library (1894)
University of Puget Sound Collins Memorial Library (1938)
University of Puget Sound School of Law Library (1978)

### Vancouver

Fort Vancouver Regional Library (1962)

### Walla Walla

Whitman College Penrose Memorial Library (1890)

## WEST VIRGINIA

### Athens

Concord College Library (1924)

### Bluefield

Bluefield State College Hardway Library (1972)

### Charleston

Kanawha County Public Library (1952)
West Virginia Library Commission (1975)
West Virginia Supreme Court Law Library (1977)

### Elkins

Davis and Elkins College Library (1913)

### Fairmont

Fairmont State College Library (1884)

### Glenville

Glenville State College Robert F. Kidd Library (1966)

### Huntington

Marshall University James E. Morrow Library (1925)

### Institute

West Virginia State College Drain-Jordon Library (1907)

### Montgomery

West Virginia Institute of Technology Vining Library (1985)

### Morgantown

West Virginia University Library (1907) REGIONAL

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Salem College Library (1921)

### Shepherdstown

Shepherd College Ruth Scarborough Library (1971)

### Weirton

Mary H. Weir Public Library (1963)

## WISCONSIN

### Appleton

Lawrence University Seeley G. Mudd Library (1869)

### Beloit

Beloit College Col. Robert H. Morse Library (1888)

### Eau Claire

University of Wisconsin-Eau Claire William D. McIntyre Library (1951)

### Fond du Lac

Fond du Lac Public Library (1966)

### Green Bay

University of Wisconsin-Green Bay Learning Resources Center (1968)

### La Crosse

La Crosse Public Library (1883)
University of Wisconsin-La Crosse Murphy Library (1965)

### Madison

Madison Public Library (1965)
State Historical Society of Wisconsin Library (1870) REGIONAL
University of Wisconsin-Madison Memorial Library (1939)
University of Wisconsin-Madison Law Library (1981)
Wisconsin State Law Library (unknown)

### Milwaukee

Alverno College Library/Media Center (1971)
Medical College of Wisconsin, Inc. Todd Wehr Library (1980)
Milwaukee County Law and Reference Library (1934)
Milwaukee Public Library (1861) REGIONAL
Mount Mary College Haggerty Library (1964)
University of Wisconsin-Milwaukee Library (1960)

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University of Wisconsin-Platteville Karrman Library (1964)

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Superior Public Library (1908)
University of Wisconsin-Superior Jim Dan Hill Library (1935)

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Waukesha Public Library (1966)

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Marathon County Public Library (1971)

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University of Wisconsin-Whitewater Harold Anderson Library (1963)

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Natrona County Public Library (1929)

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Wyoming State Law Library (1977)
Wyoming State Library (unknown) REGIONAL

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Campbell County Public Library (1980)

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University of Wyoming, Coe Library (1907)
University of Wyoming Law Library (1978)

### Powell

Northwest Community College John Taggart Hinckley Library (1967)

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Central Wyoming College Library (1969)

### Rock Springs

Western Wyoming Community College Library (1969)

### Sheridan

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